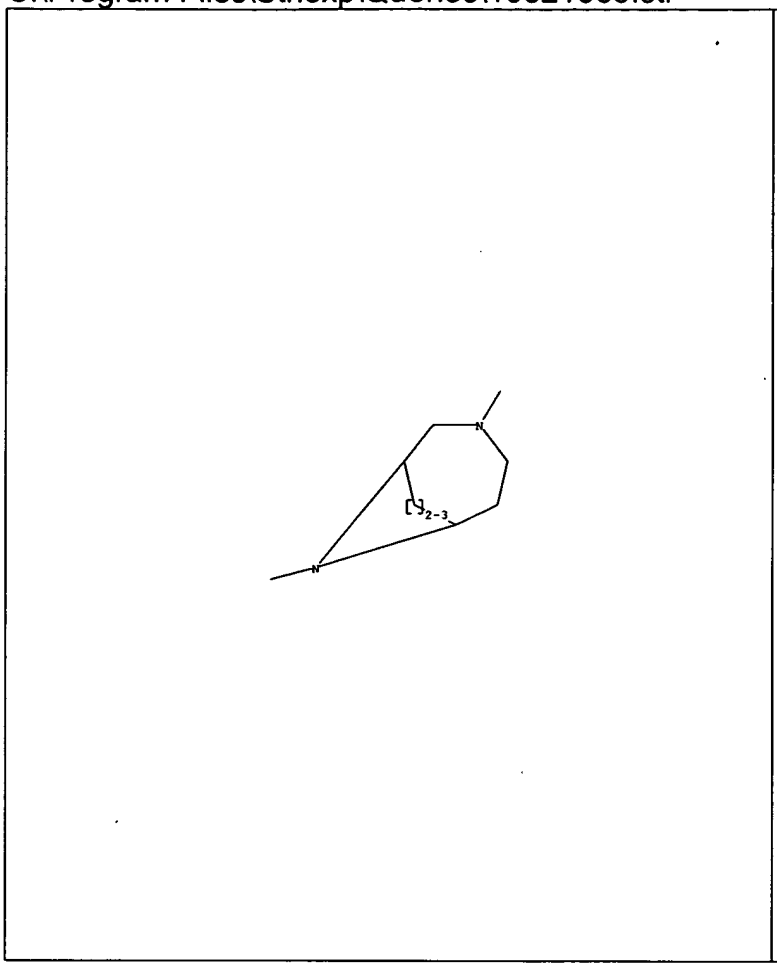
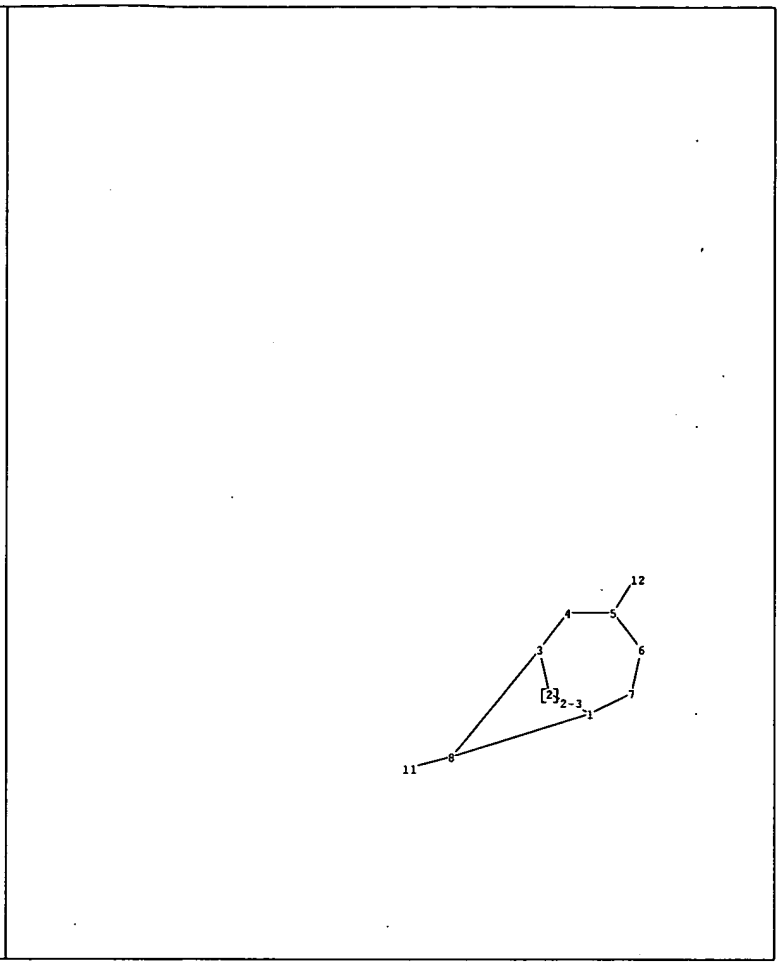
C:\Program Files\Stnexp\Queries\10521559.str





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11 12
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
5-12 8-11
ring bonds :
1-2 1-7 1-8 2-3 3-4 3-8 4-5 5-6 6-7
exact/norm bonds :
1-2 1-7 1-8 2-3 3-4 3-8 4-5 5-6 5-12 6-7 8-11

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 11:CLASS 12:CLASS

```
=> d his

     (FILE 'HOME' ENTERED AT 20:38:05 ON 30 JAN 2007)

     FILE 'REGISTRY' ENTERED AT 20:38:16 ON 30 JAN 2007
L1                STRUCTURE UPLOADED
L2                QUE L1
L3              4 S L2
L4                STRUCTURE UPLOADED
L5                QUE L4
L6              4 S L5
L7            640 S L2 SSS FUL
L8            141 S L5  SUB=L7 FUL
L9            114 S L8 AND CAPLUS/LC
L10            27 S L8 NOT L9

     FILE 'CAPLUS' ENTERED AT 20:41:32 ON 30 JAN 2007
L11            20 S L8

=> d l2
L2 HAS NO ANSWERS
L1                STR
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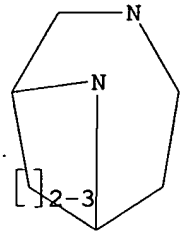


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Structure attributes must be viewed using STN Express query preparation.
L2                QUE  ABB=ON  PLU=ON  L1


=> d l5
L5 HAS NO ANSWERS
L4                STR
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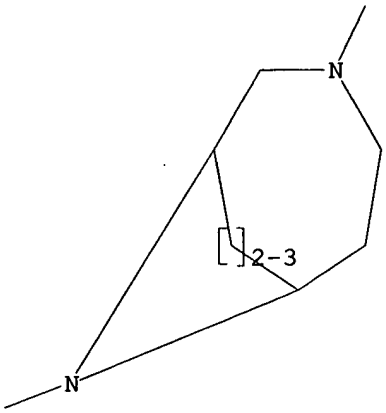


Structure attributes must be viewed using STN Express query preparation.
L5 QUE ABB=ON PLU=ON L4

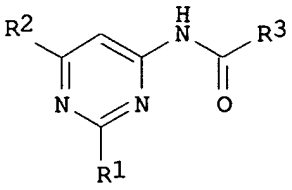
=> d ibib abs hitstr total

L1 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1093757 CAPLUS
DOCUMENT NUMBER: 145:438634
TITLE: Preparation of acylaminopyrimidines as adenosine receptor antagonists
INVENTOR(S): Slee, Deborah; Lanier, Marion; Vong, Binh G.; Chen, Yongsheng; Zhang, Xiaohui; Lin, Emily; Moorjani, Manisha; Castro Palomino Laria, Julio Cesar
PATENT ASSIGNEE(S): Neurocrine Biosciences, Inc., USA; Almirall Prodesfarma, S.A.
SOURCE: PCT Int. Appl., 172pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006110884	A2	20061019	WO 2006-US13940	20060411
WO 2006110884	A3	20061123		
WO 2006110884	A8	20061214		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-670482P P 20050411
OTHER SOURCE(S): MARPAT 145:438634
GI



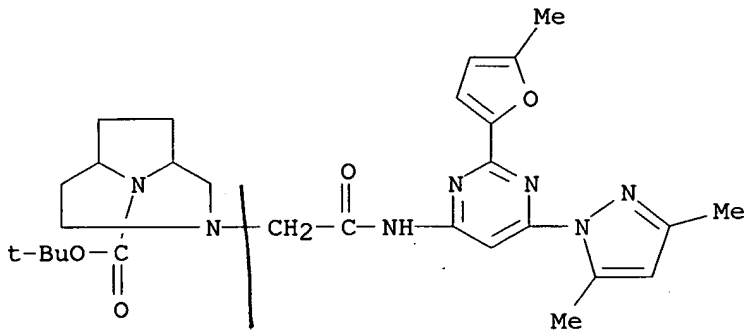
I

AB Title compds. [I; R1, R2 = (substituted) aryl, heteroaryl; R3 = (CR4R5)nR6, (CR4R5)nNR7R8, O(CR4R5)nR6, (CR4R5)nOR8; R4, R5 = H, OH, SH, NO2, cyano, amino, halo, (substituted) alkyl, alkoxy, alkylthio, cycloalkyl, alkylamino; R6 = (substituted) heterocyclyl; R7 = H, (substituted) alkyl; R8 = (CR4R5)nR6; NR7R8 = (substituted) heterocyclyl; n = 0-4], were prepared Thus, 1-tert-butoxycarbonylpiperidin-4-ylacetic acid was stirred 30 min. with (COCl)2 and cat. DMF in THF to give a first

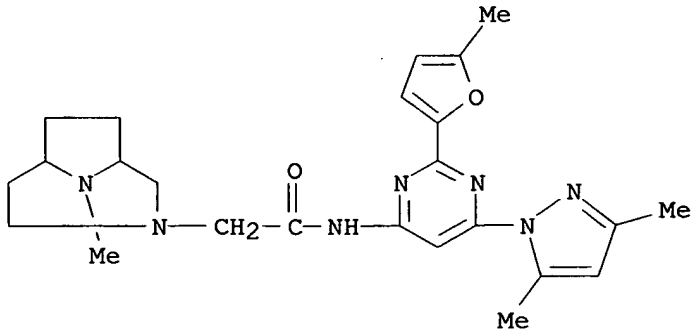
mixture; 2-(5-methyl-2-furyl)-6-(thiazol-2-yl)pyrimidin-4-amine (preparation given) in THF was treated with NaH and this second mixture was added dropwise to the first. mixture followed by stirring for 1 h to give coupling product, which was treated with CF3CO2H in CH2Cl2 to give N-[2-(5-methylfuran-2-yl)-6-thiazol-2-ylpyrimidin-4-yl]-2-(1-methylpiperidin-4-yl)acetamide. In adenosine A2A receptor binding assays, I may have IC50's of <10 μM.

IT 912939-22-1P 912939-23-2P 912939-25-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of acylaminopyrimidines as adenosine receptor antagonists)

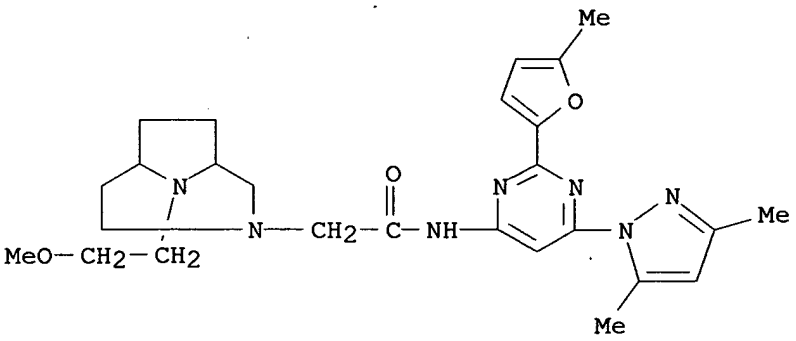
RN 912939-22-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-9-carboxylic acid, 3-[2-[[6-(3,5-dimethyl-1H-pyrazol-1-yl)-2-(5-methyl-2-furanyl)-4-pyrimidinyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 912939-23-2 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-acetamide, N-[6-(3,5-dimethyl-1H-pyrazol-1-yl)-2-(5-methyl-2-furanyl)-4-pyrimidinyl]-9-methyl- (9CI) (CA INDEX NAME)



RN 912939-25-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-acetamide, N-[6-(3,5-dimethyl-1H-pyrazol-1-yl)-2-(5-methyl-2-furanyl)-4-pyrimidinyl]-9-(2-methoxyethyl)- (9CI) (CA INDEX NAME)


Me
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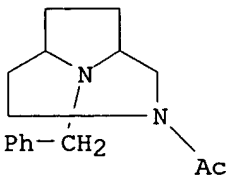
N
N
N
O
N
CH2
C
NH
N
N
Me
MeO
CH2
CH2
Me

L1 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:427357 CAPLUS
DOCUMENT NUMBER: 145:124531
TITLE: New Ligands with Affinity for the α4β2 Subtype of Nicotinic Acetylcholine Receptors. Synthesis, Receptor Binding, and 3D-QSAR Modeling
AUTHOR(S): Audouze, Karine; Oestergaard Nielsen, Elsebet; Olsen, Gunnar M.; Ahring, Philip; Jorgensen, Tino Dyhring; Peters, Dan; Liljefors, Tommy; Balle, Thomas
CORPORATE SOURCE: NeuroSearch A/S, Ballerup, DK-2750, Den.
SOURCE: Journal of Medicinal Chemistry (2006), 49(11), 3159-3171
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124531

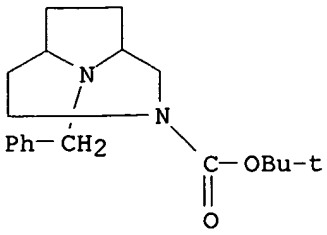
AB A new series of piperazines, diazepanes, diazocanes, diazabicyclononanes, and diazabicyclodecanes with affinity for the α4β2 subtype of nicotinic acetylcholine receptors were synthesized on the basis of results from a previous computational study. A predictive 3D-QSAR model was developed using the GRID/GOLPE approach (R2 = 0.94, Q2 = 0.83, SDEP = 0.34). The SAR was interpreted in terms of contour maps of the PLS coeffs. and in terms of a homol. model of the α4β2 subtype of the nicotinic acetylcholine receptors. The results reveal that hydrogen bonding from both hydrogens on the protonated amine and from the pyridine nitrogen to a water mol. as well as van der Waals interactions between the substituent bearing the protonated amine and the receptor is of importance for ligand affinity. The combination of 3D-QSAR and homol. modeling proved successful for the interpretation of structure-affinity relationships as well as the validation of the individual modeling approaches.

IT 387870-06-6P 653600-90-9P 897396-22-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, receptor binding, and 3D-QSAR modeling of new ligands with affinity for the α4β2 subtype of nicotinic acetylcholine receptors)

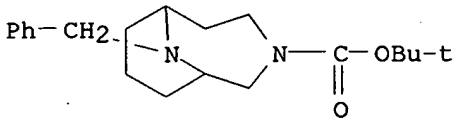
RN 387870-06-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-acetyl-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 653600-90-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 897396-22-4 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane-3-carboxylic acid, 10-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

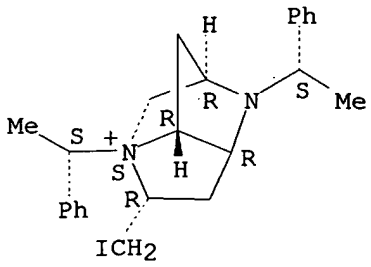
L11 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1082696 CAPLUS
DOCUMENT NUMBER: 144:6754
TITLE: Iodine-mediated cyclization of (4R,5R)-4,5-diamino-N,N'-bis[(1S)-1-phenylethyl]-1,7-octadiene - a stereoselective route to 2,5-diazabicyclo[2.2.1]heptanes
AUTHOR(S): Fiorelli, Claudio; Marchioro, Carla; Martelli, Gianluca; Monari, Magda; Savoia, Diego
CORPORATE SOURCE: Dipartimento di Chimica "G. Ciamician", Universita di Bologna, Bologna, 40126, Italy
SOURCE: European Journal of Organic Chemistry (2005), (18), 3987-3993
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:6754

AB Treatment of (4R,5R)-4,5-diamino-N,N'-bis[(1S)-1-phenylethyl]-1,7-octadiene with 2 equivalent of iodine in CH2Cl2/aqueous NaHCO3 gave a mixture of two quaternary ammonium salts in 70:30 ratio and almost quant. yield. The structure of the prevalent salt was determined by X-ray anal., which showed a bridged diazatricyclic skeleton, derived from two iodoamination steps, both involving the 5-exo cyclization of two 5-aminoalkene moieties, and an intramol. substitution involving the amine and iodide functions. The minor salt is an isomer of the prevalent one, formed by a pathway involving the stereospecific isomerization of the diastereomeric (iodomethyl)pyrrolidine produced in the first step to an (iodo)piperidine derivative via an aziridinium intermediate. Treatment of both products with different reagents, including (isopropyl)magnesium chloride, BuLi, Bu3SnH·Et3B, Cr(OAc)2 and Na2S2O4, invariably gave the bridged piperazine (1S,3R,4S)-3-allyl-2,5-bis[(1S)-1-phenylethyl]-2,5-diazabicyclo[2.2.1]heptane by a retro reaction, and hydrogenolysis of the N-substituents and concomitant hydrogenation of the C=C bond were then achieved in the presence of Pd/C.

IT 869895-79-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (iodomethyl)(aza)(azonia)tricyclononane derivative and study of its conversion to 2,5-diazabicyclo[2.2.1]heptane and study of its crystal and mol. structures)

RN 869895-79-4 CAPLUS
CN 2H-1,5-Methanopyrrolo[3,2-b]pyrrolium, hexahydro-2-(iodomethyl)-1,4-bis[(1S)-1-phenylethyl]-, iodide, (1S,2R,3aR,5R,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



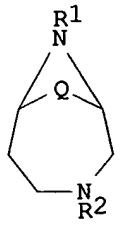
● I^-

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:101167 CAPLUS
DOCUMENT NUMBER: 140:146174
TITLE: Preparation of diazabicyclononanes and -decanes as opioid receptor ligands.
INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elseber Ostegaard
PATENT ASSIGNEE(S): Neurosearch A/S, Den.
SOURCE: PCT Int. Appl., 22 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004011468	A1	20040205	WO 2003-DK510		20030724
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2489165	A1	20040205	CA 2003-2489165		20030724
AU 2003280306	A1	20040216	AU 2003-280306		20030724
EP 1527075	A1	20050504	EP 2003-771053		20030724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1668621	A	20050914	CN 2003-817282		20030724
JP 2005536522	T	20051202	JP 2004-523742		20030724
NZ 537182	A	20060728	NZ 2003-537182		20030724
US 2005239773	A1	20051027	US 2005-521559		20050119
PRIORITY APPLN. INFO.:			DK 2002-1143	A	20020726
			WO 2003-DK510	W	20030724

OTHER SOURCE(S): MARPAT 140:146174
GI



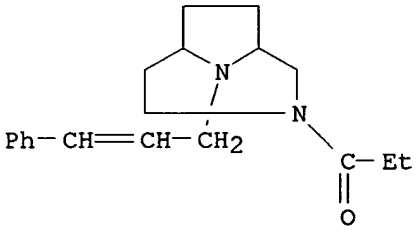
I

AB Title compds. [I; Q = CH2CH2, CH2CH2CH2; 1 of R1, R2 = (CH2)3R3, CH2CH:CHR3, CH2C.tplbond.CR3, the other = COR4; R3 = (substituted) aryl, heteroaryl; R4 = alkyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl], were prepared Thus,1-[9H-3,9-diazabicyclo[4.2.1]non-3-yl]propan-1-one (preparation

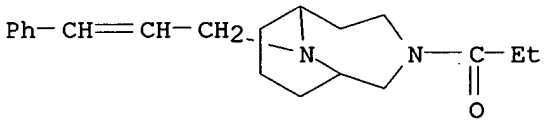
given), K2CO3, and cinnamyl bromide were stirred 15 h in acetone to give 49% 1-[9-(3-phenylallyl)-3,9-diazabicyclo[4.2.1]non-3-yl]propan-1-one hydrochloride. The latter at 10 μM showed 51% and 78% inhibition of δ- and κ-receptors, resp.

IT 653600-80-7P 653600-81-8P 653600-82-9P
653600-83-0P 653600-84-1P 653600-85-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diazabicyclononanes and -decanes as opioid receptor ligands)

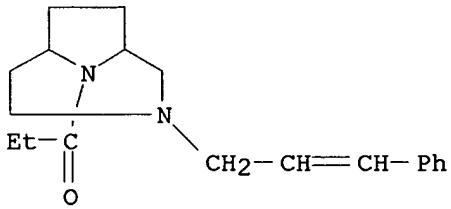
RN 653600-80-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(1-oxopropyl)-9-(3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



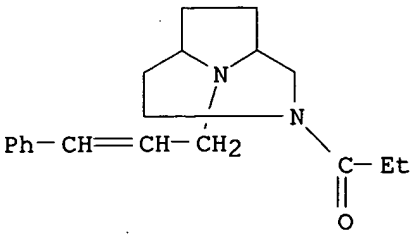
RN 653600-81-8 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(1-oxopropyl)-10-(3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



RN 653600-82-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-(1-oxopropyl)-3-(3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



RN 653600-83-0 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(1-oxopropyl)-9-(3-phenyl-2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

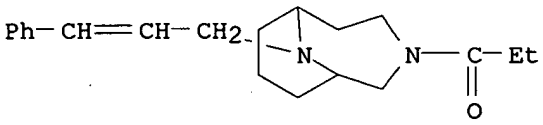


● HCl

RN 653600-84-1 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(1-oxopropyl)-10-(3-phenyl-2-propenyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

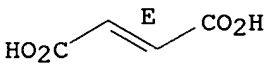
CRN 653600-81-8
CMF C20 H28 N2 O



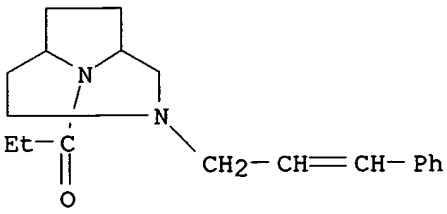
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



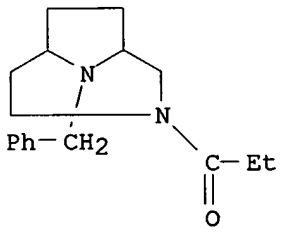
RN 653600-85-2 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-(1-oxopropyl)-3-(3-phenyl-2-propenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



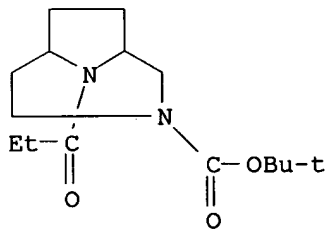
● HCl

IT 653600-87-4P 653600-89-6P 653600-90-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diazabicyclononanes and -decanes as opioid receptor ligands)

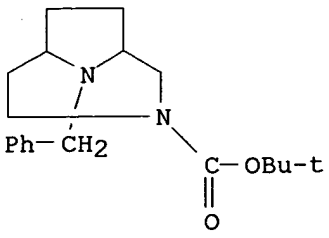
RN 653600-87-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(1-oxopropyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 653600-89-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-(1-oxopropyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 653600-90-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

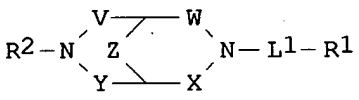


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

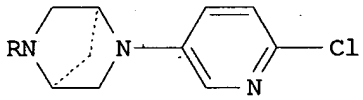
L11 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:950110 CAPLUS
DOCUMENT NUMBER: 140:16752
TITLE: Preparation of diazabicyclic central nervous system (CNS) active agents for use in pharmaceutical compositions
INVENTOR(S): Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 49 pp., Cont. of U.S. Ser. No. 466,719.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2003225268	A1	20031204	US 2003-412510		20030411
PRIORITY APPLN. INFO.:			US 1999-117807P	P	19990129
			US 1999-466719	A1	19991217

OTHER SOURCE(S): MARPAT 140:16752
GI



I



II

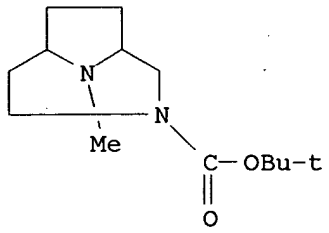
AB Diazabicyclic compds., such as I [V and X = bond or CH2; W and Y = bond, CH2, or CH2CH2; Z = CH2, CH2CH2, or CH2CH2CH2; L1 = a bond or (CH2)n; n = 1-5; R1 = heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R2 = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH2], were prepared for therapeutic use controlling synaptic transmission in mammals. These diazabicycles are claimed for use in the treatment of Alzheimer's disease, Parkinson's disease, memory dysfunction, Tourette's syndrome, sleep disorders, attention deficit hyperactivity disorder, neurodegeneration, inflammation, neuroprotection, amyotrophic lateral sclerosis, anxiety, depression, mania, schizophrenia, anorexia and other eating disorders, AIDS-induced dementia, epilepsy, urinary incontinence, Crohn's disease, migraines, premenstrual syndrome, erectile dysfunction, substance abuse, smoking cessation, and inflammatory bowel syndrome. Thus, (1S,4S)-2-(6-chloro-3-pyridinyl)-2,5-diazabicyclo[2.2.1]heptane II (R = H) was prepared via a reaction of tert-Bu (1S,4S)-2,5-diazabicyclo[2.2.1]heptane-2-carboxylate with 2-chloro-5-iodopyridine using tert-BuONa, Pd2(dba)3 and BINAP in toluene to give the BOC-protected intermediate II (R = CO2CMe3) in 58% yield and subsequent N-deprotection of II (R = CO2CMe3) using 4N HCl/dioxane to form II (R = H) in 77% yield. The prepared diazabicycles were assayed for nicotinic acetylcholine receptor binding potency in synaptic membrane prepns. from whole rat brain and were

tested for their effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents in the mouse hot plate paradigm.

IT 286947-15-7P, tert-Butyl 9-methyl-3,9-diazabicyclo[4.2.1]nonane-3-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diazabicyclic central nervous system active agents for use in pharmaceutical compns. which selectively control neurotransmitter release)

RN 286947-15-7 CAPLUS

CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

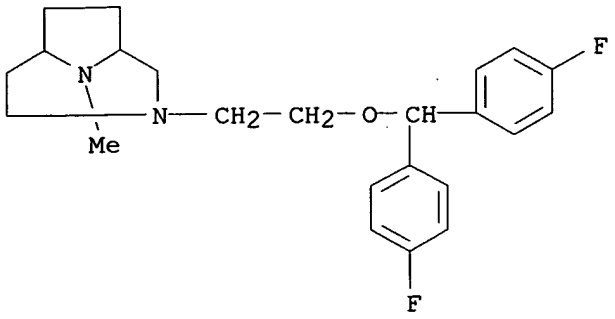


L11 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:289209 CAPLUS
DOCUMENT NUMBER: 137:195439
TITLE: Studies of the biogenic amine transporters. 10. Characterization of a novel cocaine binding site in brain membranes prepared from dopamine transporter knockout mice
AUTHOR(S): Rothman, Richard B.; Carroll, F. Ivy; Morales, Marisela; Rowley, Daniel L.; Rice, Kenner C.; Dersch, Christina M.; Donovan, David M.
CORPORATE SOURCE: IRP, NIDA, NIH, Baltimore, MD, 21224, USA
SOURCE: Synapse (New York, NY, United States) (2002), 44(2), 94-105
CODEN: SYNAET; ISSN: 0887-4476
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Previous work suggested that the cocaine analog [125I]RTI-55 labels a novel binding site in rat brain membranes, which is not associated with the dopamine (DA), serotonin (5-HT), or norepinephrine (NE) transporters. Here, we tested whether this site is a product of the DA transporter (DAT) gene. We used a T-antigen knock-in at the DAT gene that results in an effective DAT knock-out (KO) confirmed by Southern blot, DAT immunohistochem., and [125I]RTI-55 ligand binding. Brain membranes were prepared from frozen whole brain minus caudate of wild-type (WT) B6/Sv 129, +/+ and -/- (KO) mice. KO mice were used at approx. 23 days of age. Binding surface anal. of [125I]RTI-55 binding to membranes prepared from the brains of WT mice, with 100 nM citalopram to block binding to the 5-HT transporter (SERT), revealed two binding sites: the DAT and a second site, replicating previous studies conducted with rat brains. In the absence of the DAT (-/- mice), binding surface anal. demonstrated that [125I]RTI-55 labeled two sites: the NET and a second site called site "X.". Structure-activity studies of site "X" demonstrated that high-affinity ligands for the DAT, NET, and SERT have low or negligible affinity for site "X.". The relatively high d. of site "X" in brain membranes and the fact that the Ki values of cocaine and cocaethylene for site "X" are in the range achieved in the brain following cocaine administration suggests that site "X" could contribute to the pharmacol. or toxicol. effects of cocaine. Further progress in delineating the function of site "X" will depend on developing potent and selective agents for this site.

IT 321365-92-8
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel cocaine binding site in brain membranes prepared from dopamine transporter knockout mice)

RN 321365-92-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-9-methyl- (9CI) (CA INDEX NAME)



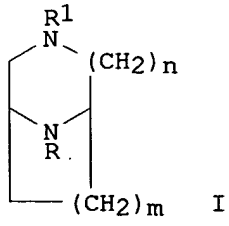
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:31453 CAPLUS
DOCUMENT NUMBER: 136:85836
TITLE: Aryl- and heteroaryl-substituted diazabicycloalkanes as cholinergic ligands for the nicotinic acetylcholine receptor
INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Ahring, Philip K.; Nielsen, Simon Feldbaek; Jorgensen, Tino Dyhring
PATENT ASSIGNEE(S): Neurosearch A/S, Den.
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002564	A1	20020110	WO 2001-DK432	20010620
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2410945	A1	20020110	CA 2001-2410945	20010620
EP 1301514	A1	20030416	EP 2001-943186	20010620
EP 1301514	B1	20050126		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502692	T	20040129	JP 2002-507816	20010620
AT 287888	T	20050215	AT 2001-943186	20010620
NZ 522793	A	20050225	NZ 2001-522793	20010620
US 2003176416	A1	20030918	US 2002-276160	20021113
US 7060699	B2	20060613		
HK 1057550	A1	20050520	HK 2004-100323	20040115

PRIORITY APPLN. INFO.:
DK 2000-1037 A 20000704
WO 2000-PA1037 A 20000704
WO 2001-DK432 W 20010620

OTHER SOURCE(S): MARPAT 136:85836
GI



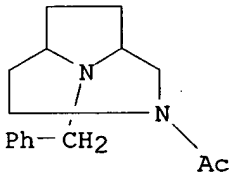
I

AB Title compds. I [one of R and R1 = H, alkyl, cycloalkyl, cycloalkylalkyl, alkenyl, alkynyl, monocyclic or polycyclic aryl, aralkyl and the other = 1 (un)substituted monocyclic or polycyclic aryl; n = 2, 3; m = 1, 2, 3] and their dimers were prepared for use as cholinergic ligands at the nicotinic acetylcholine receptors and modulators of the monoamine receptors and transporters. Thus, 9-methyl-3,9-diazabicyclo[4.2.1]nonane was treated with 2-chloroquinoline to give the 3-(2-quinolinyl) derivative which had an IC50 for inhibition of noradrenaline uptake at rat brain serotonin transporters of 0.013 μM. Due to their pharmacol. profile I may be useful for the treatment of diseases or disorders as diverse as those related to the cholinergic system of the central nervous system (CNS), the peripheral nervous system (PNS), diseases or disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neuro-degeneration, diseases or disorders related to inflammation, pain, and withdrawal symptoms caused by the termination of abuse of chemical substances.

IT 387870-06-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl- and heteroaryl-substituted diazabicycloalkanes as cholinergic ligands for the nicotinic acetylcholine receptor)

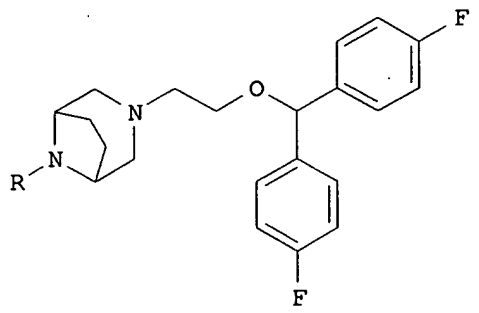
RN 387870-06-6 CAPLUS

CN 3,9-Diazabicyclo[4.2.1]nonane, 3-acetyl-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L[illegible] ANSWER 8 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:811122 CAPLUS
DOCUMENT NUMBER: 134:115932
TITLE: Synthesis and Transporter Binding Properties of Bridged Piperazine Analogues of 1-{2-[Bis(4-fluorophenyl)methoxy]ethyl}-4-(3-phenylpropyl)piperazine (GBR 12909)
AUTHOR(S): Zhang, Ying; Rothman, Richard B.; Dersch, Christina M.; de Costa, Brian R.; Jacobson, Arthur E.; Rice, Kenner C.
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases National Institutes of Health, Bethesda, MD, 20892-0815, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(25), 4840-4849
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:115932
GI

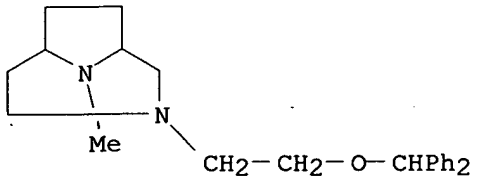


I

AB A series of bridged piperazines, e.g. I [R = Me (II), 3-phenylpropyl (III), indol-2-ylmethyl (IV), etc.], was prepared and evaluated for their ability to bind dopamine transporter (DAT) and to inhibit the uptake of 3H-labeled dopamine (DA). The binding data indicated that II and III showed high affinity for the DAT (IC50 = 8.0 and 8.2 nM, resp.), and II had high selectivity at the DAT relative to the serotonin transporter (SERT) (88- and 93-fold for binding and reuptake, resp.). II and III also displayed linear activity in DA uptake inhibition, having similar binding and reuptake inhibition profile to the title non-bridged analog (GBR 12909). Compound IV showed the highest affinity (IC50 = 1.4 nM) in the series, with a 6-fold increase over III. Interestingly, IV exhibited a high ratio (29-fold) of IC50 for the inhibition of DA reuptake vs. binding to the DAT.

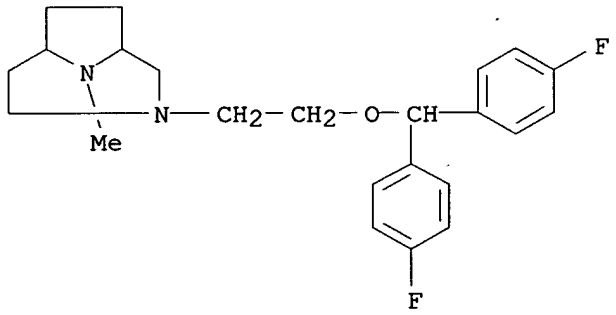
IT 321366-09-0P 321366-10-3P 321366-12-5P
321366-13-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and dopamine transporter binding properties of bridged piperazines)
RN 321366-09-0 CAPLUS

CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-(diphenylmethoxy)ethyl]-9-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



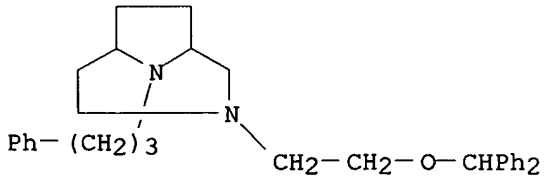
●2 HCl

RN 321366-10-3 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-9-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



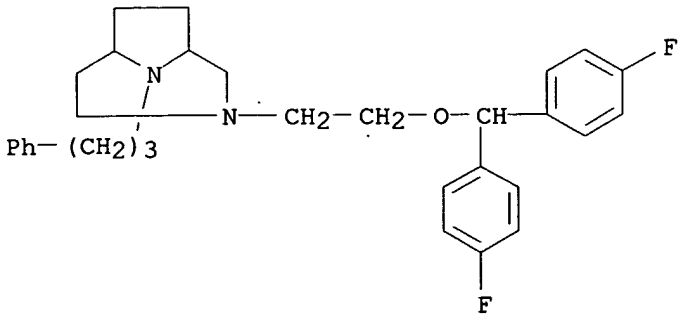
●2 HCl

RN 321366-12-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-(diphenylmethoxy)ethyl]-9-(3-phenylpropyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

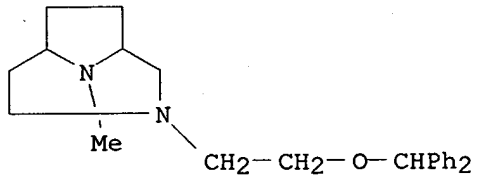
RN 321366-13-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-9-(3-phenylpropyl)-, dihydrochloride (9CI) (CA INDEX NAME)



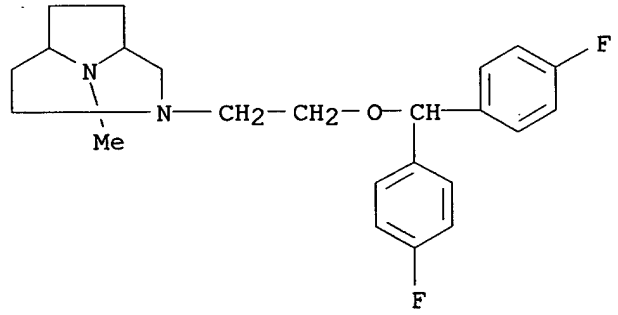
● 2 HCl

IT 321365-91-7P 321365-92-8P 321365-95-1P
321365-96-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dopamine transporter binding properties of bridged piperazines)

RN 321365-91-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-(diphenylmethoxy)ethyl]-9-methyl- (9CI) (CA INDEX NAME)

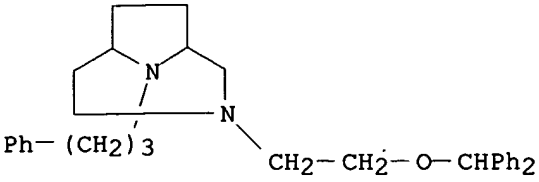


RN 321365-92-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-9-methyl- (9CI) (CA INDEX NAME)

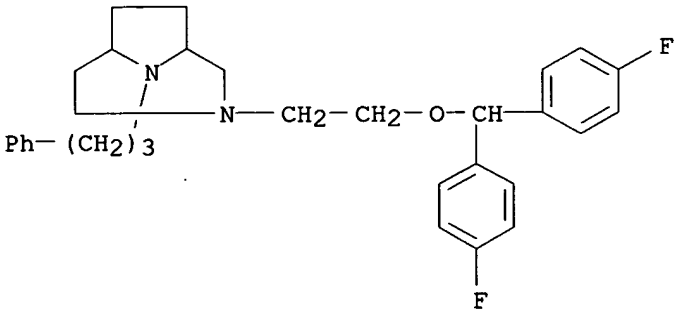


RN 321365-95-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-(diphenylmethoxy)ethyl]-9-(3-

phenylpropyl)- (9CI) (CA INDEX NAME)



RN 321365-96-2 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-9-(3-phenylpropyl)- (9CI) (CA INDEX NAME)



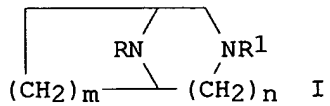
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:790504 CAPLUS
DOCUMENT NUMBER: 133:350254
TITLE: Heteroaryl diazabicycloalkanes and their affinity for nicotinic acetylcholine receptors
INVENTOR(S): Peters, Dan; Nielsen, Simon Feldbaek; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard
PATENT ASSIGNEE(S): Neurosearch A/S, Den.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066586	A1	20001109	WO 2000-DK211	20000427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2365258	A1	20001109	CA 2000-2365258	20000427
EP 1177196	A1	20020206	EP 2000-922470	20000427
EP 1177196	B1	20040310		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002543201	T	20021217	JP 2000-615616	20000427
NZ 513575	A	20030725	NZ 2000-513575	20000427
AT 261448	T	20040315	AT 2000-922470	20000427
AU 774867	B2	20040708	AU 2000-42858	20000427
US 2002037893	A1	20020328	US 2001-933944	20010822
US 6552012	B2	20030422		

PRIORITY APPLN. INFO.: DK 1999-602 A 19990504
WO 2000-DK211 W 20000427

OTHER SOURCE(S): MARPAT 133:350254
GI



I

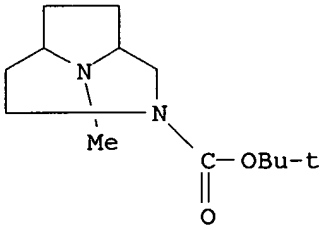
AB Title compds. I (m = 1, 2, 3; n = 2, 3; one of R and R1 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aryl, etc., and the other of R and R1 = heterocyclyl) were prepared for treatment of disorders involving nicotinic acetylcholine receptors. Thus, a mixture of 3.6 mmol 9-methyl-3,9-diazabicyclo[4.2.1]nonane, 3.6 mmol 3,6-dichloropyridazine, and 20 mL toluene was stirred at reflux for 2.5 h and the product treated with a 9:1 Et2O-MeOH mixture saturated with fumaric acid to give a 24% yield of

3-(6-chloro-3-pyridazinyl)-9-methyl-3,9-diazabicyclo[4.2.1]nonane fumaric acid salt. The affinities of I for nicotinic acetylcholine receptors were determined in tests for in vitro inhibition of 3H-epibatidin, 3H-α-bungarotoxin, and 3H-cytisine binding.

IT 286947-15-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(heteroaryl diazabicycloalkanes and their affinity for nicotinic acetylcholine receptors)

RN 286947-15-7 CAPLUS

CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

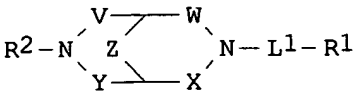


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

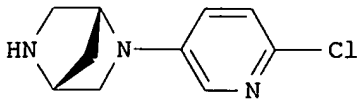
L1 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:535147 CAPLUS
DOCUMENT NUMBER: 133:135332
TITLE: Preparation of diazabicyclic derivatives as nicotinic acetylcholine receptor ligands
INVENTOR(S): Bunnelle, William H.; Cristina, Daniela Barlocco; Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy, Kevin B.; Toupence, Richard B.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 123 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044755	A1	20000803	WO 2000-US1620	20000125
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2361525	A1	20000803	CA 2000-2361525	20000125
EP 1147112	A1	20011024	EP 2000-906998	20000125
EP 1147112	B1	20031029		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200102162	T2	20011221	TR 2001-2162	20000125
BR 2000007664	A	20020507	BR 2000-7664	20000125
HU 200200332	A2	20020629	HU 2002-332	20000125
JP 2002535409	T	20021022	JP 2000-596011	20000125
EP 1359152	A2	20031105	EP 2003-17562	20000125
EP 1359152	A3	20031217		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 253067	T	20031115	AT 2000-906998	20000125
NZ 512884	A	20040326	NZ 2000-512884	20000125
PT 1147112	T	20040331	PT 2000-906998	20000125
AU 773795	B2	20040603	AU 2000-28569	20000125
ES 2209825	T3	20040701	ES 2000-906998	20000125
CN 1636996	A	20050713	CN 2004-10097482	20000125
ZA 2001005835	A	20021016	ZA 2001-5835	20010716
NO 2001003731	A	20010918	NO 2001-3731	20010730
BG 105836	A	20020329	BG 2001-105836	20010822
HK 1043116	A1	20041015	HK 2002-102948	20020418
PRIORITY APPLN. INFO.:			US 1999-239838 A	19990129
			EP 2000-906998 A3	20000125
			WO 2000-US1620 W	20000125

OTHER SOURCE(S): MARPAT 133:135332
GI



I



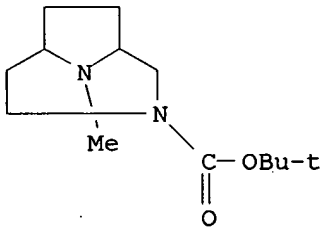
II

AB The title compds. (I) [wherein V and X = independently a bond or CH2; W and Y = independently a bond, CH2, or CH2CH2; Z = CH2, CH2CH2, or CH2CH2CH2; L1 = a bond or (CH2)n; n = 1-5; R1 = certain heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R2 = H, alkoxycarbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH2] and their pharmaceutically acceptable salts were prepared as cholinergic modulators for the treatment of pain and other conditions. For example, (-)-II•Ts-OH was prepared in a multi-step sequence involving N-protection of (1R,4R)-2-benzyl-2,5-diazabicyclo[2.2.1]heptane•2HBr with CO(OBu-t)2 (94%), debenzylation (93%), addition of 2-chloro-5-iodopyridine (67%), and deprotection followed by salt formation (71%). (-)-II•Ts-OH exhibited high affinity for the nicotinic acetylcholine receptor with Ki of 0.01 nM and showed a significant antinociceptive effect at the minimally ED of 0.62 μmol/kg in the mouse hot plate paradigm.

IT 286947-15-7P, tert-Butyl 9-methyl-3,9-diazabicyclo[4.2.1]nonane-3-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addition of haloheterocycles to protected diazabicyloalkanes followed by deprotection and optional substitution)

RN 286947-15-7 CAPLUS

CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

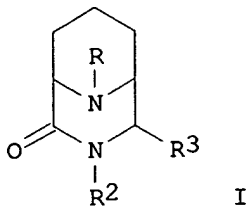


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:68456 CAPLUS
DOCUMENT NUMBER: 132:107945
TITLE: Preparation of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors
INVENTOR(S): Katoh, Susumu; Kawakami, Hiroshi; Tada, Hiroki; Linton, Maria Angelica; Kalish, Vincent; Tatlock, John Howard; Villafranca, J. Ernest
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000004020	A1	20000127	WO 1999-US15965		19990715
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2337377	A1	20000127	CA 1999-2337377		19990715
AU 9949963	A	20000207	AU 1999-49963		19990715
AU 756912	B2	20030123			
EP 1098897	A1	20010516	EP 1999-934043		19990715
EP 1098897	B1	20040609			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
BR 9912423	A	20010605	BR 1999-12423		19990715
TR 200100122	T2	20010821	TR 2001-200100122		19990715
SI 20638	A	20020228	SI 1999-20067		19990715
EE 200100032	A	20020617	EE 2001-32		19990715
JP 2002520413	T	20020709	JP 2000-560126		19990715
HU 200200637	A2	20020828	HU 2002-637		19990715
NZ 509211	A	20021025	NZ 1999-509211		19990715
AT 268772	T	20040615	AT 1999-934043		19990715
PT 1098897	T	20041029	PT 1999-934043		19990715
ES 2226409	T3	20050316	ES 1999-934043		19990715
US 6630472	B1	20031007	US 1999-356240		19990716
ZA 2001000320	A	20020711	ZA 2001-320		20010111
IN 2001MN00041	A	20050304	IN 2001-MN41		20010111
NO 2001000191	A	20010316	NO 2001-191		20010112
LT 4850	B	20011025	LT 2001-12		20010215
BG 105268	A	20011130	BG 2001-105268		20010216
HR 2001000118	A1	20020228	HR 2001-118		20010216
LV 12665	B	20011120	LV 2001-23		20010313
PRIORITY APPLN. INFO.:			US 1998-93299P	P	19980717
			US 1999-132884P	P	19990506
			WO 1999-US15965	W	19990715

OTHER SOURCE(S): MARPAT 132:107945
GI



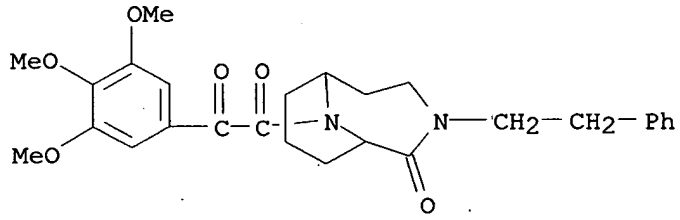
I

AB Title compds. [I; R = COCOR1; R1 = H, (cyclo)alk(en)yl, aryl, etc.; R2 = H, (ar)alkyl, alkoxy(alkyl), alkanoyloxy(alkyl), etc.; R3 = H, cyano, alkoxy, etc.; R2R3 = atoms to complete a ring] were prepared Thus, piperidine-2,6-dicarboxylic acid was N-protected and the product treated with Ac2O to give the anhydride which was cyclocondensed with PhCH2OCH2CH2NH2 to give, in 3 addnl. steps, I (R2 = CH2CH2OCH2Ph, R3 = H)(II; R = H) which was N-acylated by 3,4,5-(MeO)3C6H2COCO2H to give II [R = COCOC6H2(OMe)3-3,4,5]. Data for biol. activity of I were given.

IT 255910-70-4P 255910-71-5P 255910-72-6P
255910-76-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors)

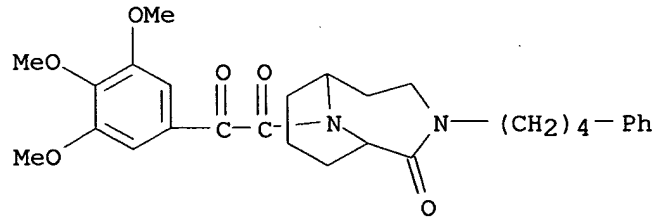
RN 255910-70-4 CAPLUS

CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



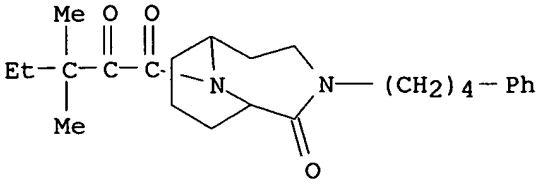
RN 255910-71-5 CAPLUS

CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

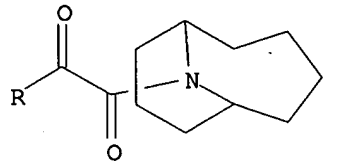


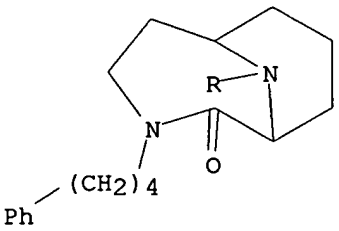
RN 255910-72-6 CAPLUS

CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-(3,3-dimethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



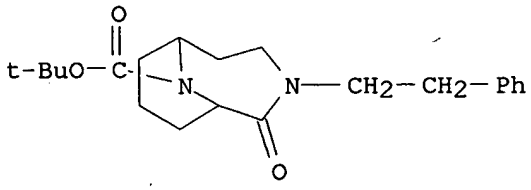
RN 255910-76-0 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-(10-azabicyclo[4.3.1]dec-10-yloxoacetyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)





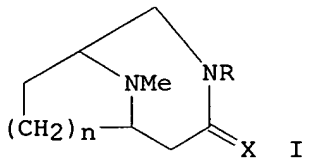
IT 255910-96-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors)

RN 255910-96-4 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane-10-carboxylic acid, 2-oxo-3-(2-phenylethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L41 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:492845 CAPLUS
DOCUMENT NUMBER: 109:92845
TITLE: Studies on azabicyclo systems. Syntheses and spasmolytic activity of analogs of 9-methyl-3,9-diazabicyclo[4.2.1]nonane and 10-methyl-3,10-diazabicyclo[4.3.1]decane
AUTHOR(S): Razdan, Balkishen; Sharma, Ashok K.; Kumari, Kanya; Bodla, Ramesh B.; Gupta, Bharat L.; Patnaik, Gyanendra K.
CORPORATE SOURCE: Dep. Pharm. Sci., Birla Inst. Technol., Mesra, 835215, India
SOURCE: European Journal of Medicinal Chemistry (1987), 22(6), 573-7
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:92845
GI



I

AB Diazabicyclo compds. I (n = 1, 2; x = H2, R = H) were prepared and converted to amides, e.g., I [n = 1, 2; x = H2, R = COR1; R1 = Me, CH2Cl, Et, Pr, Ph, substituted Ph, CH2CH2Cl, (CH2)mNR2R3; m = 2, 3; R2 = H, R3 = Et, Ph, 2-MeC6H4, 4-MeC6H4; NR2R3 = piperidino, morpholino] and sulfonamides I [n = 1, 2, X = H, R = SO2R4; R4 = Ph, 4-MeC6H4, 4-H2NC6H4). All the compds. prepared and I (n = 1, 2; X = O, R = H) were tested for spasmolytic activity. I (n = 1, X = H2, R = H; II) showed specific anti-serotonin activity. Amides of II with aromatic acids showed antihistaminic properties whereas amides of I (n = 2, X = H2, R = H) with aliphatic acids showed spasmogenic activity. A number of amides and sulfonamides showed non-specific spasmolytic activity.

IT 115748-53-3P 115748-54-4P 115748-55-5P
115748-56-6P 115748-57-7P 115748-58-8P
115748-59-9P 115748-60-2P 115748-61-3P
115748-62-4P 115748-63-5P 115748-64-6P
115748-65-7P 115748-66-8P 115748-68-0P
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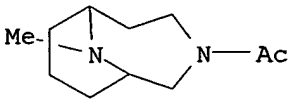
115748-99-7P 115749-00-3P 115749-01-4P
115749-02-5P 115749-03-6P 115749-04-7P
115749-05-8P 115749-06-9P 115749-07-0P
115749-08-1P 115749-09-2P 115749-10-5P
115749-11-6P 115791-76-9P 115791-77-0P
115791-78-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and spasmolytic activity of)

RN 115748-53-3 CAPLUS

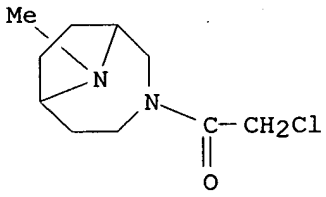
CN 3,10-Diazabicyclo[4.3.1]decane, 3-acetyl-10-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 115748-54-4 CAPLUS

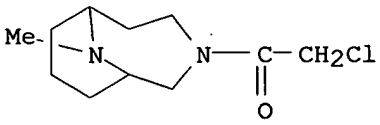
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(chloroacetyl)-9-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 115748-55-5 CAPLUS

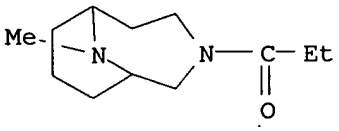
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(chloroacetyl)-10-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

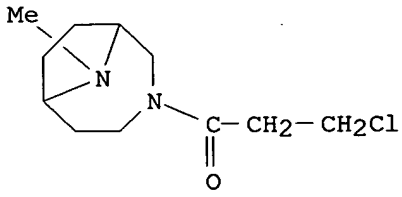
RN 115748-56-6 CAPLUS

CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-oxopropyl)-, monohydrochloride (9CI) (CA INDEX NAME)



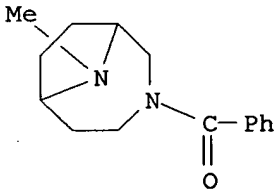
● HCl

RN 115748-57-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(3-chloro-1-oxopropyl)-9-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



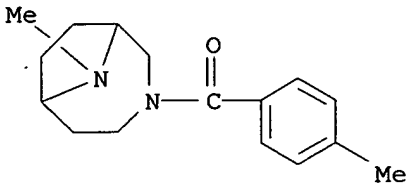
● HCl

RN 115748-58-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-benzoyl-9-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



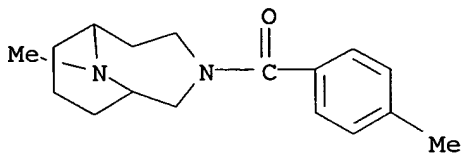
● HCl

RN 115748-59-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(4-methylbenzoyl)-, monohydrochloride (9CI) (CA INDEX NAME)



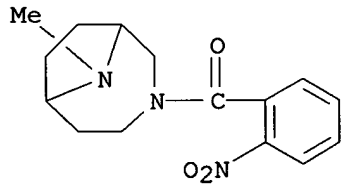
● HCl

RN 115748-60-2 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(4-methylbenzoyl)-, monohydrochloride (9CI) (CA INDEX NAME)



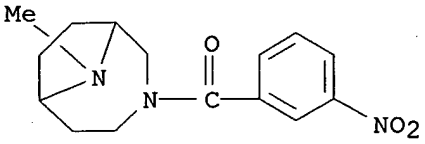
● HCl

RN 115748-61-3 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(2-nitrobenzoyl)-, monohydrochloride (9CI) (CA INDEX NAME)



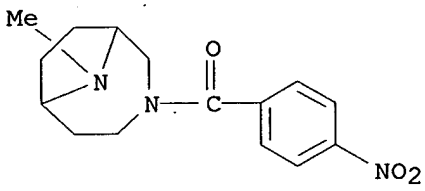
● HCl

RN 115748-62-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(3-nitrobenzoyl)-, monohydrochloride (9CI) (CA INDEX NAME)



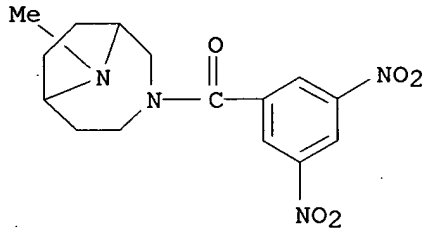
● HCl

RN 115748-63-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(4-nitrobenzoyl)-, monohydrochloride (9CI) (CA INDEX NAME)



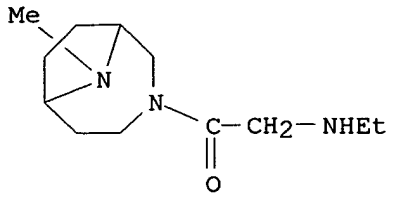
● HCl

RN 115748-64-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(3,5-dinitrobenzoyl)-9-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



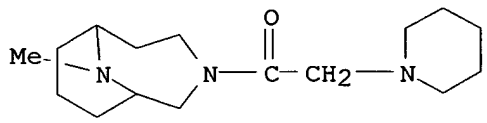
● HCl

RN 115748-65-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[(ethylamino)acetyl]-9-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 115748-66-8 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-piperidinylacetyl)-, dihydrochloride (9CI) (CA INDEX NAME)

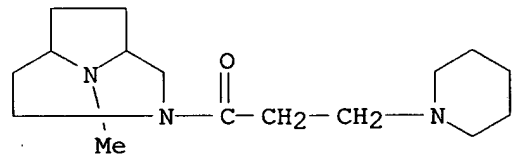


●2 HCl

RN 115748-68-0 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[1-oxo-3-(1-piperidinyl)propyl]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

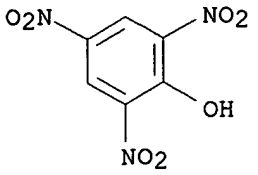
CM 1

CRN 115748-67-9
CMF C16 H29 N3 O

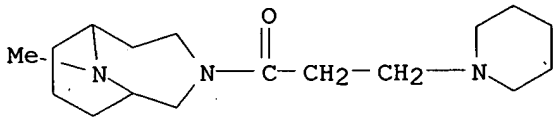


CM 2

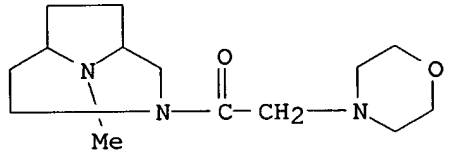
CRN 88-89-1
CMF C6 H3 N3 O7



RN 115748-69-1 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-[1-oxo-3-(1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)



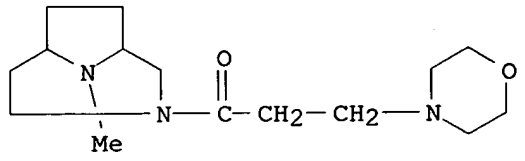
RN 115748-70-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(4-morpholinylacetyl)- (9CI) (CA INDEX NAME)



RN 115748-72-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-(4-morpholinyl)-1-oxopropyl]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

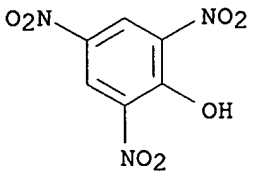
CM 1

CRN 115748-71-5
CMF C15 H27 N3 O2



CM 2

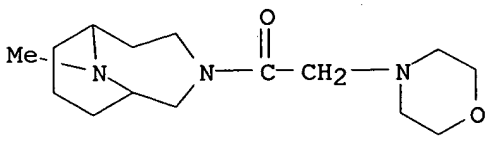
CRN 88-89-1
CMF C6 H3 N3 O7



RN 115748-74-8 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(4-morpholinylacetyl)-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

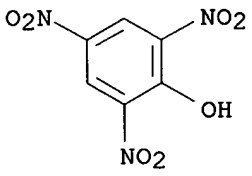
CM 1

CRN 115748-73-7
CMF C15 H27 N3 O2

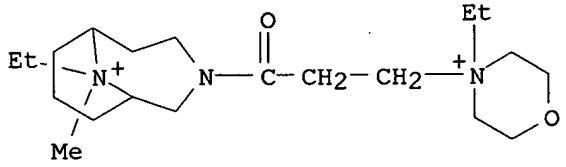


CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



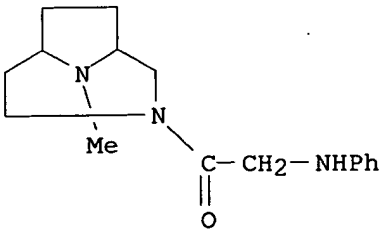
RN 115748-75-9 CAPLUS
CN 3-Aza-10-azoniabicyclo[4.3.1]decane, 10-ethyl-3-[3-(4-ethylmorpholinium-4-yl)-1-oxopropyl]-10-methyl-, diiodide (9CI) (CA INDEX NAME)



●2 I⁻

RN 115748-76-0 CAPLUS

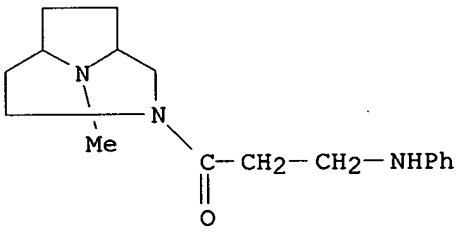
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[(phenylamino)acetyl]- (9CI) (CA INDEX NAME)



RN 115748-78-2 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[1-oxo-3-(phenylamino)propyl]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

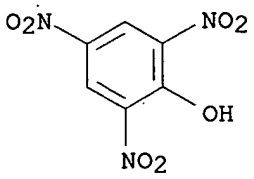
CM 1

CRN 115748-77-1
CMF C17 H25 N3 O

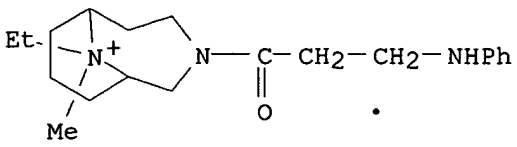


CM 2

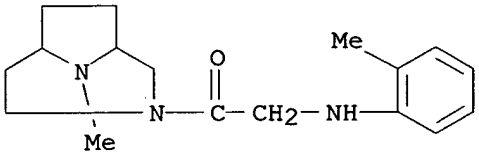
CRN 88-89-1
CMF C6 H3 N3 O7



RN 115748-79-3 CAPLUS
CN 3-Aza-10-azoniabicyclo[4.3.1]decane, 10-ethyl-10-methyl-3-[1-oxo-3-(phenylamino)propyl]-, iodide (9CI) (CA INDEX NAME)



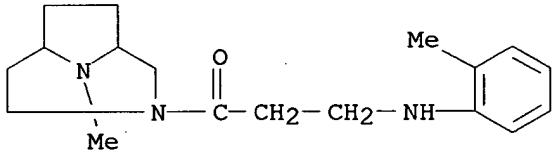
RN 115748-80-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[[(2-methylphenyl)amino]acetyl]-(9CI) (CA INDEX NAME)



RN 115748-82-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-[(2-methylphenyl)amino]-1-oxopropyl]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

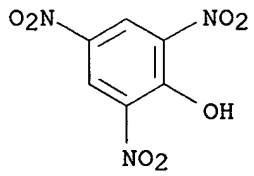
CM 1

CRN 115748-81-7
CMF C18 H27 N3 O

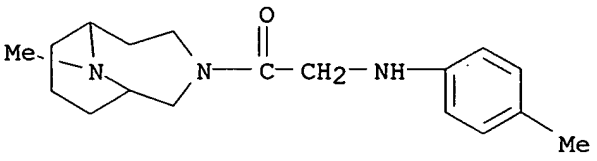


CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



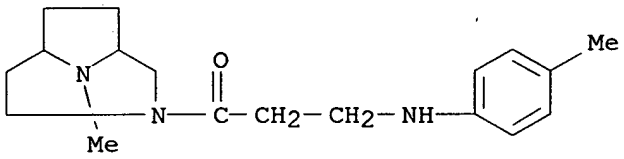
RN 115748-83-9 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-[[(4-methylphenyl)amino]acetyl]- (9CI) (CA INDEX NAME)



RN 115748-85-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-[(4-methylphenyl)amino]-1-oxopropyl]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

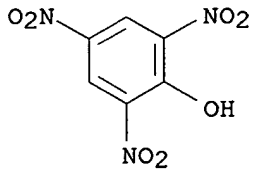
CM 1

CRN 115748-84-0
CMF C18 H27 N3 O

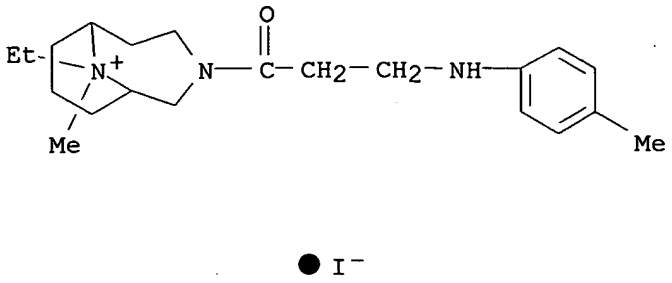


CM 2

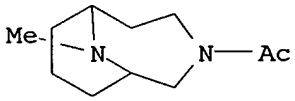
CRN 88-89-1
CMF C6 H3 N3 O7



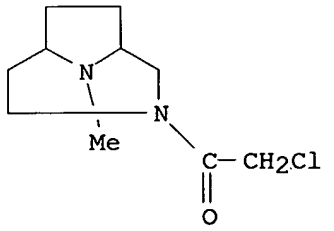
RN 115748-86-2 CAPLUS
CN 3-Aza-10-azoniabicyclo[4.3.1]decane, 10-ethyl-10-methyl-3-[3-[(4-methylphenyl)amino]-1-oxopropyl]-, iodide (9CI) (CA INDEX NAME)



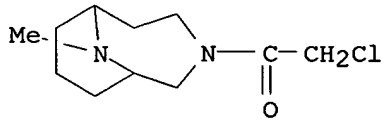
RN 115748-97-5 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-acetyl-10-methyl- (9CI) (CA INDEX NAME)



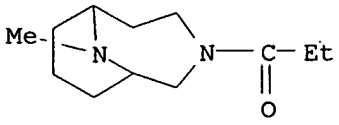
RN 115748-98-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(chloroacetyl)-9-methyl- (9CI) (CA INDEX NAME)



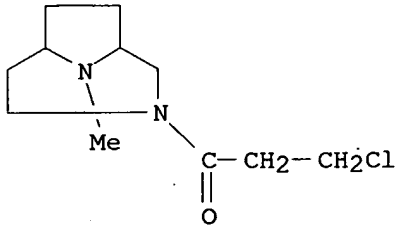
RN 115748-99-7 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(chloroacetyl)-10-methyl- (9CI) (CA INDEX NAME)



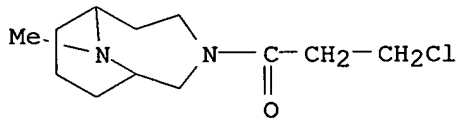
RN 115749-00-3 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-oxopropyl)- (9CI) (CA INDEX NAME)



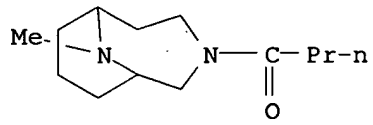
RN 115749-01-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(3-chloro-1-oxopropyl)-9-methyl- (9CI) (CA INDEX NAME)



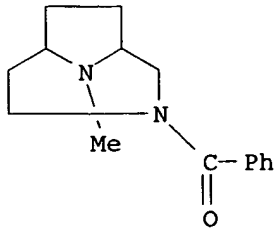
RN 115749-02-5 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(3-chloro-1-oxopropyl)-10-methyl- (9CI) (CA INDEX NAME)



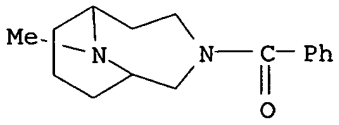
RN 115749-03-6 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-oxobutyl)- (9CI) (CA INDEX NAME)



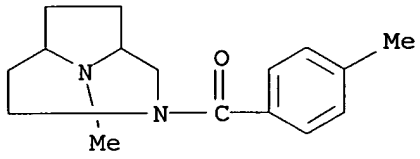
RN 115749-04-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-benzoyl-9-methyl- (9CI) (CA INDEX NAME)



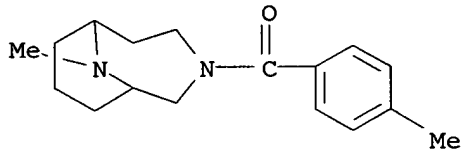
RN 115749-05-8 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-benzoyl-10-methyl- (9CI) (CA INDEX NAME)



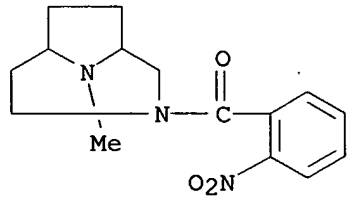
RN 115749-06-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



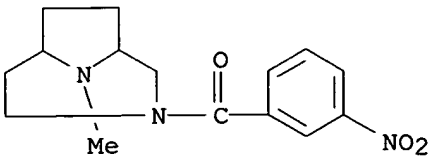
RN 115749-07-0 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



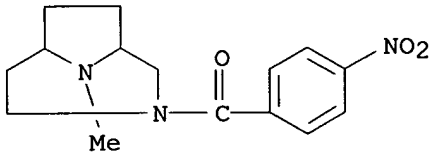
RN 115749-08-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(2-nitrobenzoyl)- (9CI) (CA INDEX NAME)



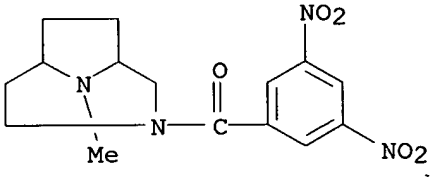
RN 115749-09-2 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(3-nitrobenzoyl)- (9CI) (CA INDEX NAME)



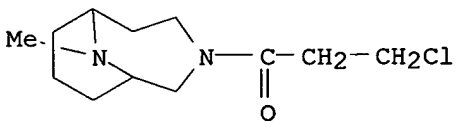
RN 115749-10-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(4-nitrobenzoyl)- (9CI) (CA INDEX NAME)



RN 115749-11-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(3,5-dinitrobenzoyl)-9-methyl- (9CI) (CA INDEX NAME)

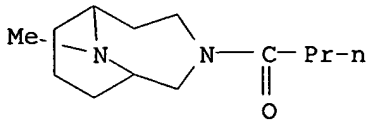


RN 115791-76-9 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-(3-chloro-1-oxopropyl)-10-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



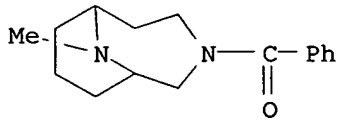
● HCl

RN 115791-77-0 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-oxobutyl)-, monohydrochloride (9CI) (CA INDEX NAME)



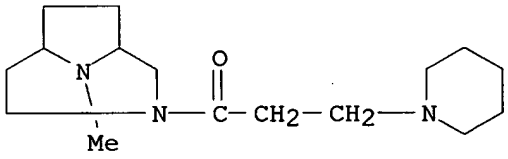
● HCl

RN 115791-78-1 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 3-benzoyl-10-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

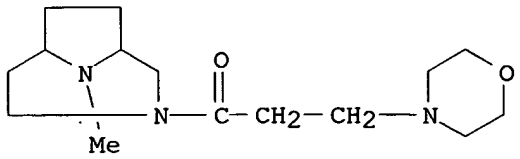


● HCl

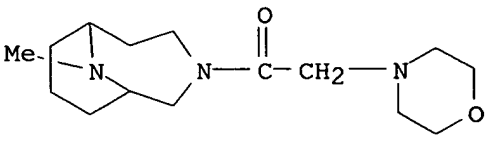
IT 115748-67-9P 115748-71-5P 115748-73-7P
115748-77-1P 115748-81-7P 115748-84-0P
115748-93-1P 115748-94-2P 115748-95-3P
115748-96-4P 115791-79-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 115748-67-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[1-oxo-3-(1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)



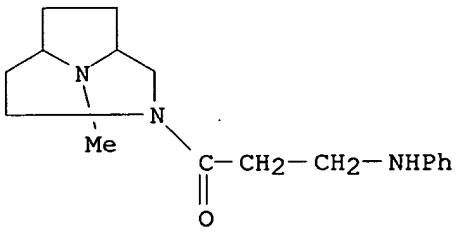
RN 115748-71-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-(4-morpholinyl)-1-oxopropyl]- (9CI) (CA INDEX NAME)



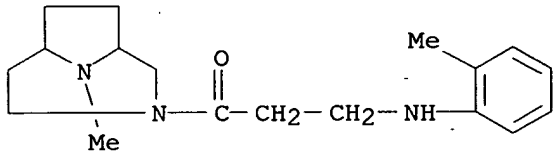
RN 115748-73-7 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(4-morpholinylacetyl)- (9CI) (CA INDEX NAME)



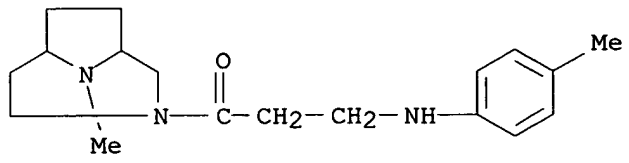
RN 115748-77-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[1-oxo-3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)



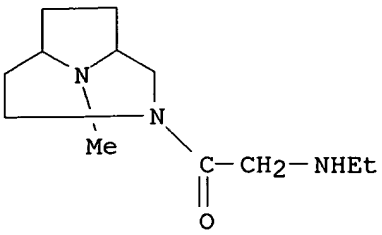
RN 115748-81-7 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-[(2-methylphenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



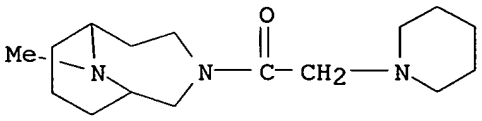
RN 115748-84-0 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-[3-[(4-methylphenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



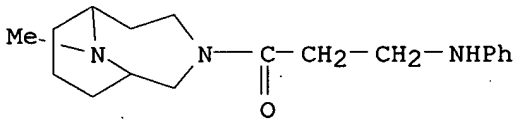
RN 115748-93-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[(ethylamino)acetyl]-9-methyl- (9CI) (CA INDEX NAME)



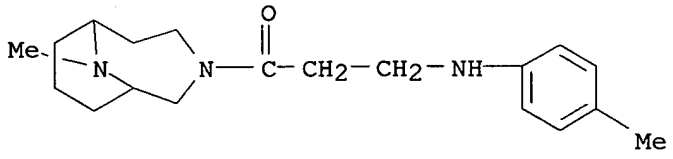
RN 115748-94-2 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-(1-piperidinylacetyl)- (9CI) (CA INDEX NAME)



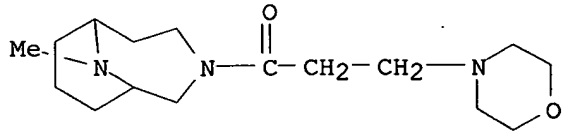
RN 115748-95-3 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-[1-oxo-3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)



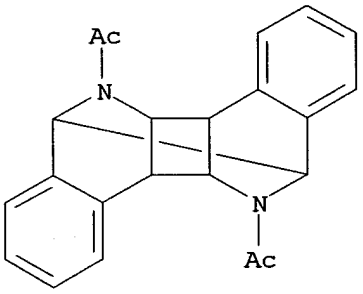
RN 115748-96-4 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-[3-[(4-methylphenyl)amino]-1-oxopropyl]- (9CI) (CA INDEX NAME)



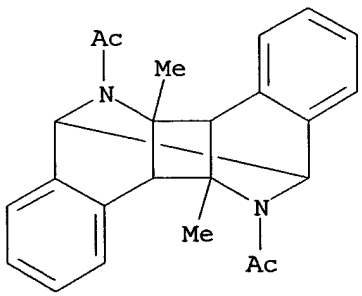
RN 115791-79-2 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decane, 10-methyl-3-[3-(4-morpholinyl)-1-oxopropyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:89650 CAPLUS
DOCUMENT NUMBER: 86:89650
TITLE: Photoreactions. 47. Internal photocyclization of bis(1,2-dihydroisoquinolines) and a methylenebis(naphthalenone)
AUTHOR(S): Nakamura, Yushin; Zsindely, Janos; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Heterocycles (1976), 5(1), 427-43
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The racemic isoquinoline dimers I (R = H, Me) underwent photocycloaddn. to give II (R = H, Me, R1 = Ac), which were reduced with (Me2CHCH2)2AlH2 to give II (R1 = Et). Meso-I similarly gave III, together with II (R = Me, R1 = AC). The naphthalenone dimer IV similarly gave V.
IT 61876-92-4P 61876-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 61876-92-4 CAPLUS
CN 6,11,13-(Iminometheno)-5H-dibenzo[a,e]cyclononen-5,12-imine, 15,16-diacetyl-6,11,12,13-tetrahydro- (9CI) (CA INDEX NAME)



RN 61876-98-0 CAPLUS
CN 6,11,13-(Iminometheno)-5H-dibenzo[a,e]cyclononen-5,12-imine, 15,16-diacetyl-6,11,12,13-tetrahydro-12,14-dimethyl- (9CI) (CA INDEX NAME)

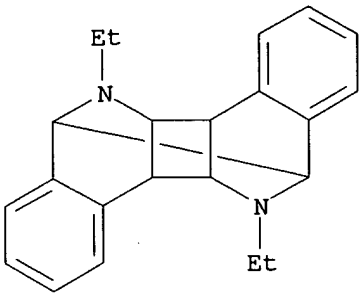


IT 61876-93-5P 61876-99-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

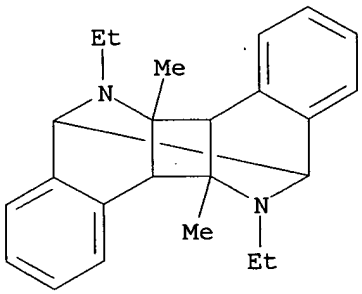
RN 61876-93-5 CAPLUS

CN 6,11,13-(Iminometheno)-5H-dibenzo[a,e]cyclononen-5,12-imine, 15,16-diethyl-6,11,12,13-tetrahydro- (9CI) (CA INDEX NAME)

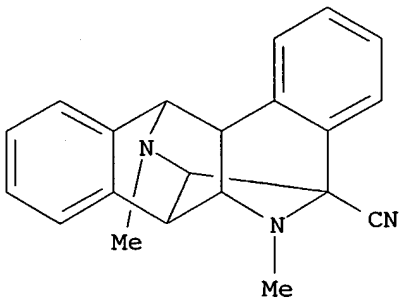


RN 61876-99-1 CAPLUS

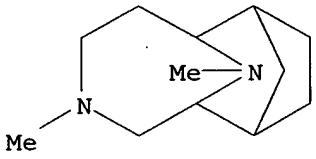
CN 6,11,13-(Iminometheno)-5H-dibenzo[a,e]cyclononen-5,12-imine, 15,16-diethyl-6,11,12,13-tetrahydro-12,14-dimethyl- (9CI) (CA INDEX NAME)



L11 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:461757 CAPLUS
DOCUMENT NUMBER: 77:61757
TITLE: Alkylation, acylation, and reduction studies on 1-cyano-1,2-dihydro- and -1,2,3,4-tetrahydroisoquinoline derivatives
AUTHOR(S): Boehme, Horst; Stoecker, Klaus Peter
CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Marburg, Marburg/L., Fed. Rep. Ger.
SOURCE: Chemische Berichte (1972), 105(5), 1578-85
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Successive treatment of 2-benzoyl-1-cyano-1,2,3,4-tetrahydroisoquinoline (I) with NaH in DMF and with alkyl or acyl halides gave the corresponding 1-alkyl- or 1-acyl-1-cyano-1,2,3,4-tetrahydroisoquinolines (II), resp. Thioacylation and cyanoethylation of I with PhNCS and CH2:CHCN, resp., also took place in 1-position. Reduction of 2-alkyl-1-cyano-1,2-dihydroisoquinolines with LiAlH4 gave 2-alkyl-1,2-dihydro-isoquinolines (III).
IT 37039-55-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 37039-55-7 CAPLUS
CN 12,5,7-(Iminometheno)benzo[b]phenanthridine-5(6H)-carbonitrile, 6a,7,12,12a-tetrahydro-6,13-dimethyl- (9CI) (CA INDEX NAME)

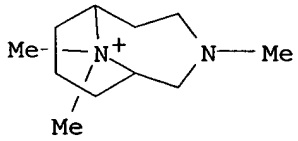


L11 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:488799 CAPLUS
DOCUMENT NUMBER: 75:88799
TITLE: Synthesis and some conformational observations on the 3,10-diazabicyclo[4.3.1]decane system
AUTHOR(S): Sasaki, Tadashi; Eguchi, Shoji; Kiriyama, Tsutomu
CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, Japan
SOURCE: Journal of Organic Chemistry (1971), 36(15), 2061-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 10-Methyl-3,10-diazabicyclo[4.3.1]decane (I) and its 7.9-exo-ethano derivative were prepared by LiAlH4 reduction of 10-methyl-3.10-diazabicyclo[4.3.1]decan-4-one (II) and its 7,9-cxo-ethano derivative (III), both of which were obtained by the Schmidt reaction of pseudopelletierine (IV) and 6,8-exo-ethanopseudopelletierine (V), resp. The same reduction of II afforded 76% stable Al complex, tris(10-methyl-3,10-diazabicyclo[4.3.1]decane)alum inum hydroxide, but reduction of III yielded no such stable complex. Treatment of I with 1 equivalent of methylene iodide gave 10-methyl-3,10-diazatricyclo[4.3.1.13,10]undecanium iodide (19).
IT 29577-65-9P 29584-56-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29577-65-9 CAPLUS
CN 8,11-Diazatricyclo[4.4.1.12,5]dodecane, 8,11-dimethyl-, monohydriodide, stereoisomer (8CI) (CA INDEX NAME)



● HI

RN 29584-56-3 CAPLUS
CN 3-Aza-10-azoniabicyclo[4.3.1]decane, 3,10,10-trimethyl-, iodide (8CI) (CA INDEX NAME)



● I⁻

L11 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:43499 CAPLUS
DOCUMENT NUMBER: 72:43499
TITLE: Tranquilizing N-(aroylalkyl)azabicycloalkanes
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: Fr., 20 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

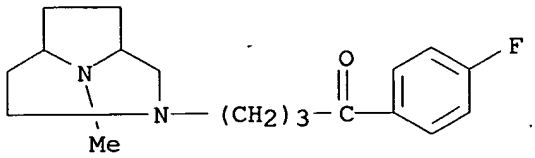
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1549235		19681213	FR	19670720
CH 486463			CH	
CH 508626			CH	
DE 1670448			DE	
FR 7320			FR	
GB 1195729			GB	
PRIORITY APPLN. INFO.:			CH	19660727
			CH	19670606

OTHER SOURCE(S): MARPAT 72:43499
GI For diagram(s), see printed CA Issue.
AB The title compds. I or II were prepared To 20 g 3-azabicyclo[3.2.2]nonane (III), 50.4 g Na2CO3 and some crys ts. of KI in 1400 ml PhMe was added 44.8 g p-FC6H4CO(CH2)3Cl. The mixture was refluxed 48 hr worked up and treated with anhydrous HCl to give I (Ar = 4-FC6H4, n = 3) (Ia).HCl m. 189-90° (iso-PrOH-Et2O); Ia maleate m. 132° (MeOH-iso-PrOH). Ia.HCl was also prepared from 7.6 g 3-(3-cyanopropyl)-3-azabicyclo[3.2.2]nonane (hydrochloride m. 260°, from III, Cl(CH2)3CN, Na2CO3, and KI in PhMe) in 75 ml Et2O and 4-FC6H4MgBr from 14 g 4-FC6H4Br and 1.92 g Mg in 40 ml Et2O. Reduction of 3 g Ia.HCl by 0.3 g NaBH4 in 20 ml. 50% MeOH gave II (Ar = 4-FC6H4, n = 3), m. 70°; HCl salt m. 216-17°. Similarly prepared were the following I (n = 3) (Ar and m.p. HCl salt given). 3-CF3C6H4, 210°; 4-MeOC6H4, 188°; 2-thienyl, 220-2°; 4-PhOC6H4, 263-5°; 4-ClC6H4, 242°; 4-tert-BuC6H4, 244-5°; 3-FC6H4, - (maleate, m. 139-40°); 3-thienyl, 228°; 4-iso-PrC6H4, 243°; 4-BrC6H4, 267-8°; 3,4-Me2C6H3, 247-8°; 2,4-(MeO)2C6H3, 182-3°; Ph, 230-2° (MeOH); 4-MeC6H4, 225-6°; 2,5-Me2C6H3, 203-4°; 4-HOC6H4, 312-13° (decomposition); and 2,4-Me2C6H3, 203-4°. Also prepared were IV.HCl, m. 158-9° (hemihydrate); I (Ar = p-FC6H4, n = 4)-HCl, m. 85-6° (dihydrate) [from 3-(4-cyanobutyl)-3-azabicyclo[3.2.2]nonane, hydrochloride, m. 278-9°]; V.HCl, m. 118-20° [from 9-methyl-4-oxo-3,9-diazabicyclo[4.2.1]nonane, m. 88° (petroleum ether), hydrochloride m. 258° (decomposition), through 9-methyl-3,9-diazabicyclo[4.2.1]-nonane, dihydrochloride m. 220° (decomposition); and I [Ar = p-FC6H4,(CH2)n = CH2CHMeCH2]. HCl, m. 145-6° [from 3-(3-cyano-2-methyl-1-propyl)-3-azabicyclo[3.2.2]nonane, hydrochloride m. 256° (decomposition). To MeLi (from 0.52 g Li and 10.65 g MeI in 50 ml. Et2O) was added 8.7 g Ia in 60 ml C6H6 to give 3-[4-(4-fluorophenyl)-4-hydroxy-4-methyl-1-butyl]-3-azabicyclo[3.2.2]nonane, maleate, m. 123°. I and II have sedative, tranquilizing and antiaggressive properties.
IT 27229-18-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 27229-18-1 CAPLUS
CN Butyrophenone, 4'-fluoro-4-(9-methyl-3,9-diazabicyclo[4.2.1]non-3-yl)-, maleate (8CI) (CA INDEX NAME)

CM 1

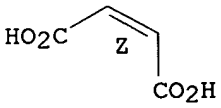
CRN 47233-13-6
CMF C18 H25 F N2 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

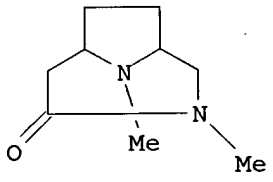


L11 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:103405 CAPLUS
DOCUMENT NUMBER: 64:103405
ORIGINAL REFERENCE NO.: 64:19371c-e
TITLE: Mass spectrometry in structural and stereochemical problems. CI. A study of the fragmentation of some azabicyclo lactams
AUTHOR(S): Duffield, A. M.; Djerassi, Carl; Wise, Lawrence; Paquette, Leo A.
CORPORATE SOURCE: Stanford Univ., Stanford, CA
SOURCE: Journal of Organic Chemistry (1966), 31(5), 1599-1602
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

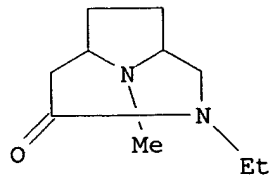
AB cf. CA 64, 5142a, 9559b, 17300c. The mass spectra of 5 azabicyclo lactams (I-V) were measured in order to examine the effect upon the fragmentation pattern of 2 different functional groups in close proximity to each other. From the utilization of deuterated analogs, supplemented by high-resolution mass spectrometry, rationalizations are presented for the principal fragments observed in the spectra of these compds. Increasing the ring size from 8 to 10 membered did not affect greatly the principal fragmentation modes.

IT 1128-77-4, 3,9-Diazabicyclo[4,2,1]nonan-4-one, 3,9-dimethyl-
7345-18-8, 3,9-Diazabicyclo[4,2,1]nonan-4-one, 3-ethyl-9-methyl-
(mass spectrum of)

RN 1128-77-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonan-4-one, 3,9-dimethyl- (7CI, 8CI) (CA INDEX NAME)



RN 7345-18-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonan-4-one, 3-ethyl-9-methyl- (7CI, 8CI) (CA INDEX NAME)

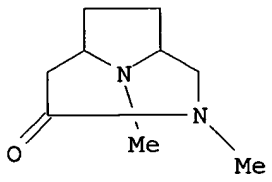


L11 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:82489 CAPLUS
DOCUMENT NUMBER: 62:82489
ORIGINAL REFERENCE NO.: 62:14645a-c
TITLE: Transannular cyclizations in medium-sized unsaturated lactams. Apparent dependence of transannular interaction upon conformational factors
AUTHOR(S): Paquette, Leo A.; Wise, Lawrence D.
CORPORATE SOURCE: Ohio State Univ., Columbus
SOURCE: Journal of the American Chemical Society (1965), 87(7), 1561-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 62:82489

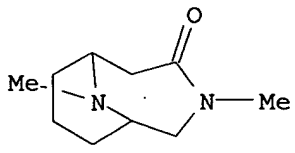
AB A series of azabicyclic amides of varying ring size (eight to ten members) are shown to be readily transformed to α,β-unsaturated lactams by the Hofmann elimination procedure. These unsaturated secondary lactams of the azacyclooctane and azacyclononane series undergo transannular cyclization when treated with acids. The related N-methylamides, as well as the azacyclodecane example, merely undergo protonation of the dimethylamino group under identical conditions. These results are discussed in terms of conformational factors.

IT 1128-77-4P, 3,9-Diazabicyclo[4,2,1]nonan-4-one, 3,9-dimethyl-
1201-54-3P, 3,10-Diazabicyclo[4.3.1]decan-4-one, 3,10-dimethyl-
1212-71-1P, 3,9-Diazabicyclo[4,2,1]nonan-4-one, 3,9-dimethyl-, perchlorate 1603-38-9P, 3-Aza-10-azoniabicyclo[4.3.1]decane, 3,10,10-trimethyl-4-oxo-, iodide
RL: PREP (Preparation)
(preparation of)

RN 1128-77-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonan-4-one, 3,9-dimethyl- (7CI, 8CI) (CA INDEX NAME)



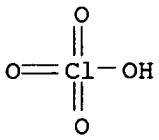
RN 1201-54-3 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-4-one, 3,10-dimethyl- (7CI, 8CI) (CA INDEX NAME)



RN 1212-71-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonan-4-one, 3,9-dimethyl-, perchlorate (7CI, 8CI) (CA INDEX NAME)

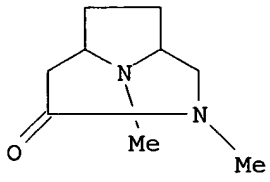
CM 1

CRN 7601-90-3
CMF Cl H O4

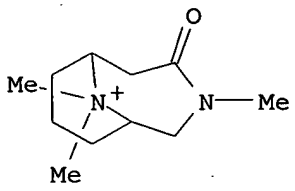


CM 2

CRN 1128-77-4
CMF C9 H16 N2 O



RN 1603-38-9 CAPLUS
CN 3-Aza-10-azoniabicyclo[4.3.1]decane, 3,10,10-trimethyl-4-oxo-, iodide (8CI) (CA INDEX NAME)



L11 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:52805 CAPLUS
DOCUMENT NUMBER: 60:52805
ORIGINAL REFERENCE NO.: 60:9297g-h,9298a-c
TITLE: 3-Acyl-9-methyl-3,9-diazabicyclo[4.2.1]nonanes
INVENTOR(S): Wagner, Hans A.
PATENT ASSIGNEE(S): G.D. Searle and Co.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3117132		19640107	US 1962-164403	19620104
PRIORITY APPLN. INFO.:			US	19620104

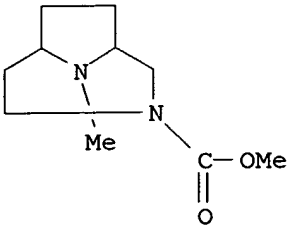
GI For diagram(s), see printed CA Issue.

AB The title compds., possessing antihypertensive, antiinflammatory, and antibacterial properties, and the ability to inhibit the incorporation of mevalonic acid during biosynthesis of cholesterol, are prepared by treating 9-methyl-3,9-diazabicyclo[4.2.1]nonane (I) with acid chlorides. Thus, 42 g. I in 500 ml. Et2O is slowly added, with vigorous agitation, to 63 g. Ph2CHCOCl in 1 l. Et2O, the mixture stirred 1 hr., the solid precipitate collected and dissolved in 500 ml. H2O, the aqueous solution adjusted to pH 8 with concentrated NaOH, the precipitated solid filtered off and taken up in Et2O, the filtrate extracted with Et2O, the combined Et2O solns. dried over CaSO4 and evaporated, and the residue recrystd. from hexane to give 9-methyl-3-diphenylacetyl-3,9-diazabicyclo [4.2.1] nonane (II), m. 106°. Similarly prepared are 3-phenylacetyl-, 3-cyclohexylacetyl-, and 3-acetoxy-9-methyl-3,9-diazabicyclo[4.2.1]nonane. I (28 g.) in 100 ml. Et2O is treated with 27 g. ClCO2-CH2CHMe2 in 250 ml. Et2O to give 3-isobutoxycarbonyl-9-methyl-3,9-diazabicyclo[4.2.1]nonane-HCl, m. 208-10° (EtOH-EtOAc). Similarly prepared is 3-(3-cyclopentylpropionyl)-9-methyl-3,9-diazabicyclo[4.2.1]nonane-HCl, m. 233° (EtOH). II (167 g.) and 139 g. p-BrC6H4COCH2Br in 2 l. EtOH is refluxed 5 hrs., allowed to stand overnight, and poured into 30 1. Et2O to precipitate 9-(p-bromobenzoylmethyl)-9-methyl-3-diphenylacetyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, m. 149° (EtOH-EtOAc). Similarly prepared were the following substituted 3-isobutoxycarbonyl-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromides (substituent and m.p. given): 9-ethoxycarbonylmethyl, .apprx.125°; 9-(p-bromobenzyl), .apprx.187°; 9-(p-bromobenzoylmethyl), .apprx.192°. Also prepared were 9,9'-p-phenylenedimethylenebis(3-isobutoxycarbonyl-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide) monohydrate, m. 172-4°; and 9,9'-o-phenylenedimethylenebis(3-isobutoxycarbonyl-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide monohydrate, m. 181-3°. Cf. Michaels and Zaugg, CA 54, 19711d.

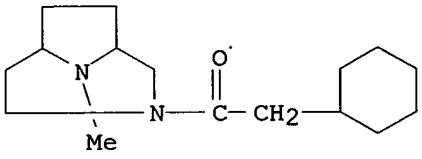
IT 91951-85-8P, 3,9-Diazahicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, methyl ester 93143-82-9P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(cyclohexylacetyl)-9-methyl- 96557-59-4P, 3,9-Diazahicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, isobutyl ester, hydrochloride 97646-22-5P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(3-cyclopentylpropionyl)-9-methyl-, hydrochloride 98068-05-4P, 3,9-Diazabicyclo[4.2.1]nonane,

9-methyl-3-(phenylacetyl)- 98271-44-4P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(diphenylacetyl)-9-methyl- 100030-08-8P, 9-(p-Bromophenacyl)-3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, isobutyl ester 100211-71-0P, 9-(p-Bromobenzyl)-3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, isobutyl ester 104016-16-2P, 9-(p-Bromophenacyl)-3-(diphenylacetyl)-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide
RL: PREP (Preparation)
(preparation of)

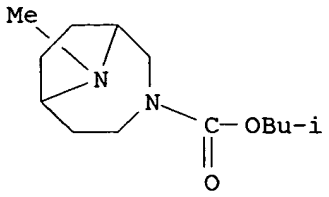
RN 91951-85-8 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, methyl ester (7CI) (CA INDEX NAME)



RN 93143-82-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(cyclohexylacetyl)-9-methyl- (7CI) (CA INDEX NAME)

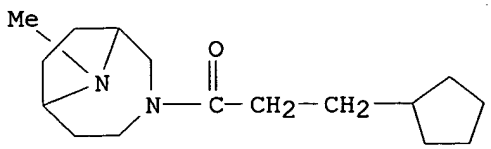


RN 96557-59-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, isobutyl ester, hydrochloride (7CI) (CA INDEX NAME)



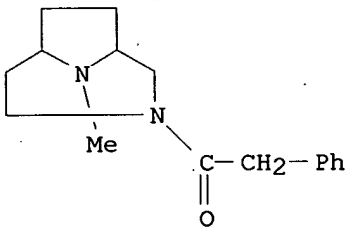
● HCl

RN 97646-22-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(3-cyclopentylpropionyl)-9-methyl-, hydrochloride (7CI) (CA INDEX NAME)

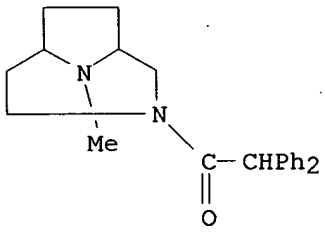


● HCl

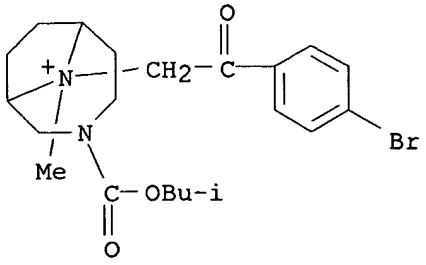
RN 98068-05-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 9-methyl-3-(phenylacetyl)- (7CI) (CA INDEX NAME)



RN 98271-44-4 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(diphenylacetyl)-9-methyl- (7CI) (CA INDEX NAME)

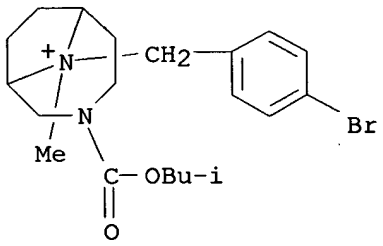


RN 100030-08-8 CAPLUS
CN 9-(p-Bromophenacyl)-3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, isobutyl ester (7CI) (CA INDEX NAME)



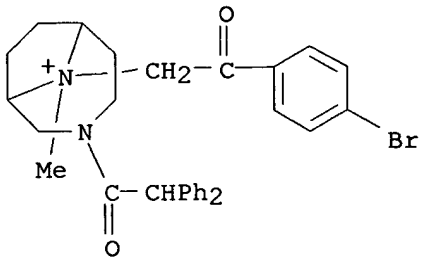
● Br^-

RN 100211-71-0 CAPLUS
CN 9-(p-Bromobenzyl)-3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, isobutyl ester (7CI) (CA INDEX NAME)



● Br^-

RN 104016-16-2 CAPLUS
CN 9-(p-Bromophenacyl)-3-(diphenylacetyl)-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide (7CI) (CA INDEX NAME)



● Br^-

L41 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:2410 CAPLUS
DOCUMENT NUMBER: 56:2410
ORIGINAL REFERENCE NO.: 56:474i,475a-d
TITLE: 3,9-Diazabicyclo[4.2.1]nonane derivatives
INVENTOR(S): Zaugg, Harold E.
PATENT ASSIGNEE(S): Abbott Laboratories
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

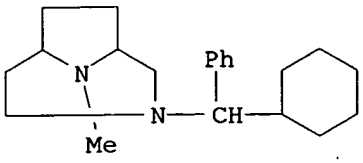
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2999091		19610905	US 1959-848235	19591023

AB 3-Tropanone (11.1 g.) in 100 ml. CHCl3, was cooled to -5° and the solution treated dropwise with 25 ml. concentrated H2SO4 below 15°. NaN3 (10.4 g.) was added in 0.5-g. portions below 35°. After the addns., which required 2 hrs., the mixture was stirred at 50° 2 hrs. The mixture was poured on ice and made alkaline with K2CO3, then 50 cc. of 60% KOH solution was added. The inorg. salts were removed by filtration and washed with CHCl3. The aqueous phase of the filtrate was extracted with CHCl3 and the combined CHCl3 solns. were dried with Na2SO4. After distillation of CHCl3 there was obtained 90% 9-methyl-3,9-diazabicyclo[4.2.1]nonan-4-one (I); HCl salt m. 258-9° (decomposition). I (11 g.) was reduced by 6.8 g. LiAlH4 in 600 ml. of Et2O at reflux for 46 hrs. to yield 68% 9-methyl-3,9-diazabicyclo[4.2.1]nonane (II), b38 111-13° n24D 1.4992; di-HCl salt m. 290-1° (decomposition). A solution of 5.9 g. p-chlorobenzhydryl chloride in 20 cc. dry xylene was added to 3.5 g. II and 4.0 g. Et3N in 70 cc. of xylene. After refluxing 22 hrs., the mixture was cooled and filtered to remove Et3N.HCl. Vacuum evaporation of xylene gave an oil, which treated with oxalic acid in ether gave 0.2 g. oxalate, which furnished 4-(p-chlorobenzhydryl)-9-methyl-4,9-diazabicyclo [4.2.1] nonane (III), m. 91°. 4-Benzhydryl-9-methyl-4,9-diazabicyclo[4.2.1]nonane (IV) was prepared by reaction of II with benzhydryl chloride. II and 9-fluorenyl chloride yielded 4-(9-fluorenyl)9-methyl-4,9-diazabicyclo[4.2.1]nonane. The halophenyl compds., 4-(p,p'-dichlorobenzhydryl)-9- methyl-4,9- diaza [4.2.1]bicyclononane (VI) and 4-(2,4-dichlorobenzhydryl)-9-methyl-4,9-diaza[4.2.1]bicyclononane (VII), are prepared, resp., by treating p,p'-dichlorobenzhydryl chloride and 2,4-dichlorobenzhydryl chloride with II. Compds. such as III-VII have ganglionic-blocking actions and are serotonin antagonists. Hydrogenation at 30 lb. H pressure and 60° with PtO2 reduced one Ph group of IV to yield 4-(cyclohexylphenylmethyl) - 9 - methyl - 4, 9 - diaza [4.2.1] bicyclononane.

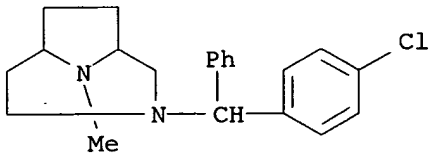
IT 94999-77-6P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(α-cyclohexylhenzyl)-9-methyl- 95005-03-1P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(p-chloro-α-phenylbenzyl)-9-methyl- 95948-57-5P, 3,9-Diazabicyclo[4.2.1]nonane, 3-[bis(p-chlorophenyl)methyl]-9-methyl- 95948-58-6P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(2,4-dichloro-α-phenylbenzyl)-9-methyl- 98131-64-7P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(diphenylmethyl)-9-methyl- 101227-56-9P, 3,9-Diazabicyclo[4.2.1]nonane, 3-(p-chloro-α-phenylbenzyl)-9-methyl-, oxalate
RL: PREP (Preparation)
(preparation of)

RN 94999-77-6 CAPLUS

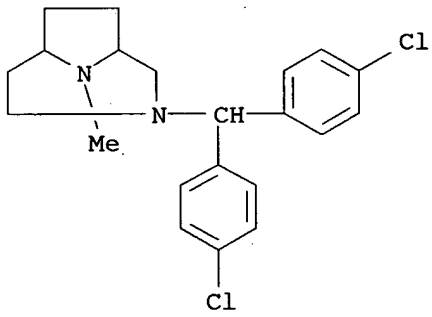
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(α-cyclohexylbenzyl)-9-methyl- (7CI) (CA INDEX NAME)



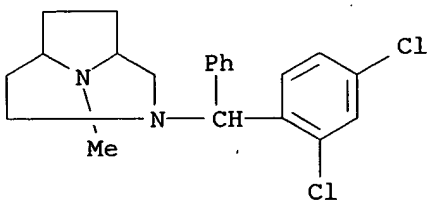
RN 95005-03-1 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(p-chloro-α-phenylbenzyl)-9-methyl- (7CI) (CA INDEX NAME)



RN 95948-57-5 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-[bis(p-chlorophenyl)methyl]-9-methyl- (7CI) (CA INDEX NAME)

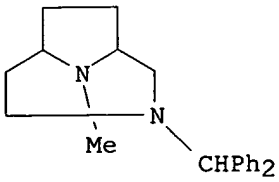


RN 95948-58-6 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(2,4-dichloro-α-phenylbenzyl)-9-methyl- (7CI) (CA INDEX NAME)



RN 98131-64-7 CAPLUS

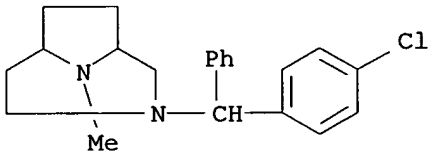
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(diphenylmethyl)-9-methyl- (7CI) (CA INDEX NAME)



RN 101227-56-9 CAPLUS
CN 3,9-Diazabicyclo[4.2.1]nonane, 3-(p-chloro-α-phenylbenzyl)-9-methyl-, oxalate (7CI) (CA INDEX NAME)

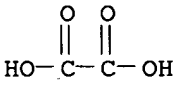
CM 1

CRN 95005-03-1
CMF C21 H25 Cl N2



CM 2

CRN 144-62-7
CMF C2 H2 O4



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L2                QUE L1
L3              4 S L2
L4                STRUCTURE UPLOADED
L5                QUE L4
L6              4 S L5
L7            640 S L2 SSS FUL
L8            141 S L5  SUB=L7 FUL
L9            114 S L8 AND CAPLUS/LC
L10            27 S L8 NOT L9

     FILE 'CAPLUS' ENTERED AT 20:41:32 ON 30 JAN 2007
L11            20 S L8

     FILE 'REGISTRY' ENTERED AT 20:42:47 ON 30 JAN 2007

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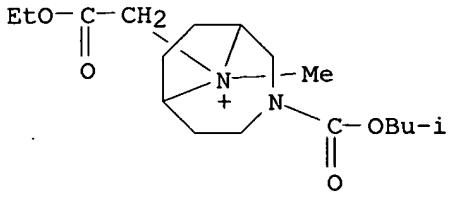
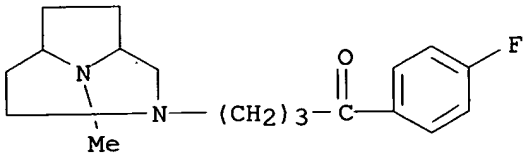
L10 ANSWER 25 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 98146-08-8 REGISTRY
ED Entered STN: 22 Sep 1985
CN 3-Carboxy-9-(carboxymethyl)-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide, 3-isobutyl ethyl ester (7CI) (CA INDEX NAME)
MF C17 H31 N2 O4 . Br
SR CAOLD
LC STN Files: CAOLD
CRN (740045-29-8)



● Br^-

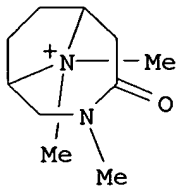
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L10 ANSWER 26 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 47233-13-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Butanone, 1-(4-fluorophenyl)-4-(9-methyl-3,9-diazabicyclo[4.2.1]non-3-yl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3,9-Diazabicyclo[4.2.1]nonane, 1-butanone deriv.
MF C18 H25 F N2 O
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 27 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 3258-76-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Aza-9-azoniabicyclo[4.2.1]nonane, 3,9,9-trimethyl-4-oxo-, iodide (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3,9,9-Trimethyl-4-oxo-3-aza-9-azoniabicyclo[4.2.1]nonane iodide (7CI)
MF C10 H19 N2 O . I
LC STN Files: CAOLD
CRN (801144-51-4)



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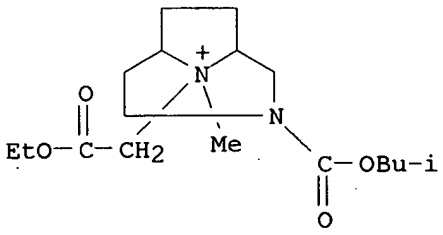
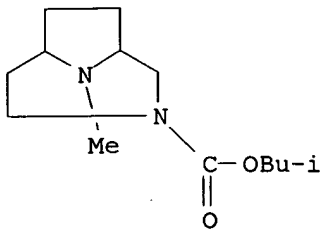
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d 110 20-24

L10 ANSWER 20 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 740045-29-8 REGISTRY
ED Entered STN: 05 Sep 2004
CN 3-Aza-9-azoniabicyclo[4.2.1]nonane, 9-(2-ethoxy-2-oxoethyl)-9-methyl-3-[(2-methylpropoxy)carbonyl]- (9CI) (CA INDEX NAME)
MF C17 H31 N2 O4
CI COM
SR CA

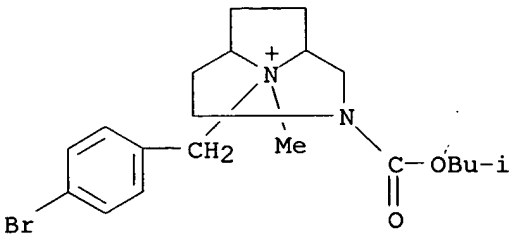


L10 ANSWER 21 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 731754-04-4 REGISTRY
ED Entered STN: 23 Aug 2004
CN 3,9-Diazabicyclo[4.2.1]nonane-3-carboxylic acid, 9-methyl-, 2-methylpropyl ester (9CI) (CA INDEX NAME)
MF C13 H24 N2 O2
CI COM
SR CA

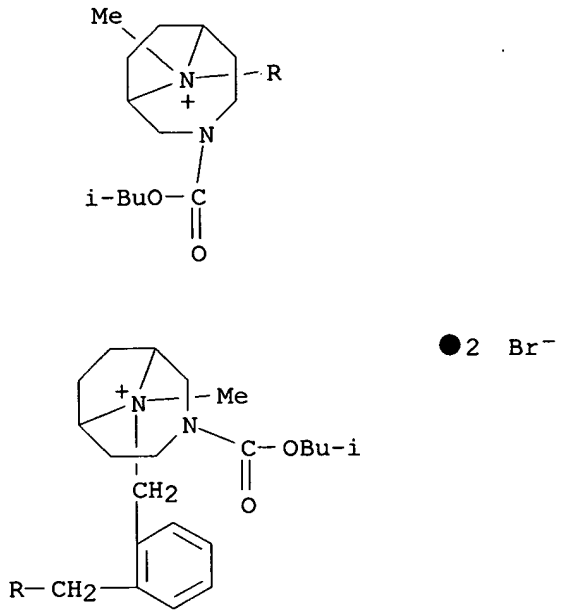


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 22 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 686257-18-1 REGISTRY
ED Entered STN: 26 May 2004
CN 3-Aza-9-azoniabicyclo[4.2.1]nonane, 9-[(4-bromophenyl)methyl]-9-methyl-3-[(2-methylpropoxy)carbonyl]- (9CI) (CA INDEX NAME)
MF C20 H30 Br N2 O2
CI COM
SR CA



L10 ANSWER 23 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 105768-22-7 REGISTRY
ED Entered STN: 21 Dec 1986
CN 9,9'-(o-Phenylenedimethylene)bis[3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide], diisobutyl ester (7CI) (CA INDEX NAME)
MF C34 H56 N4 O4 . 2 Br
SR CAOLD
LC STN Files: CAOLD
CRN (805222-36-0)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L10 ANSWER 24 OF 27 REGISTRY COPYRIGHT 2007 ACS on STN
RN 105768-21-6 REGISTRY
ED Entered STN: 21 Dec 1986
CN 9,9-(p-Phenylenedimethylene)bis[3-carboxy-9-methyl-3-aza-9-azoniabicyclo[4.2.1]nonane bromide], diisobutyl ester (7CI) (CA INDEX NAME)
MF C34 H56 N4 O4 . 2 Br
SR CAOLD
LC STN Files: CAOLD
CRN (804469-03-2)

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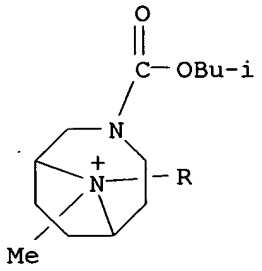

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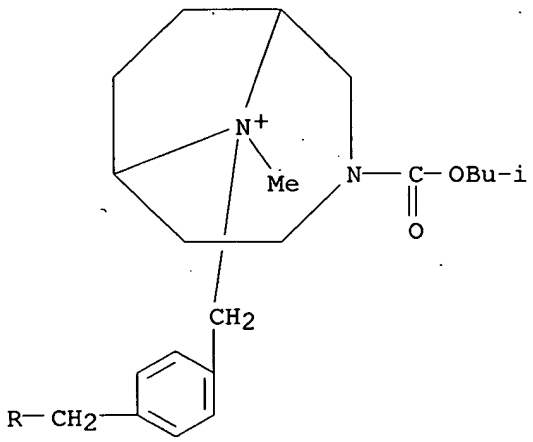

●2 Br^-

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)